On mathematical models for Bose-Einstein condensates in optical lattices (expanded version)

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Abstract

Our aim is to analyze the various energy functionals appearing in the physics literature and describing the behavior of a Bose-Einstein condensate in an optical lattice. We want to justify the use of some reduced models. For that purpose, we will use the semi-classical analysis developed for linear problems related to the Schrödinger operator with periodic potential or multiple wells potentials. We justify, in some asymptotic regimes, the reduction to low dimensional problems and analyze the reduced problems.

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*CNRS, CMAP, Ecole Polytechnique, F-91128 Palaiseau cedex, France

†Laboratoire de Mathématiques, Univ Paris-Sud et CNRS, Bat 425. 91 405 Orsay Cedex France.

1 Introduction

1.1 The physical motivation for Bose-Einstein condensates in optical lattices

Superfluidity and superconductivity are two spectacular manifestations of quantum mechanics at the macroscopic scale. Among their striking characteristics is the existence of vortices with quantized circulation. The physics of such vortices is of tremendous importance in the field of quantum fluids and extends beyond condensed matter physics. The advantage of ultracold gaseous Bose-Einstein condensates is to allow tests in the laboratory to study various aspects of macroscopic quantum physics. There is a large body of research, both experimental, theoretical and mathematical on vortices in Bose-Einstein condensates [PeSm, PiSt, Af, LSSY]. Current physical interest is in the investigation of very small atomic assemblies, for which one would have one vortex per particle, which is a challenge in terms of detection and signal analysis. An appealing option consists in parallelizing the study, by producing simultaneously a large number of micro-BECs rotating at the various nodes of an optical lattice [Sn]. Experiments are under way.

A major topic is the transition from a Mott insulator phase to a superfluid phase. We refer to the paper of Zwerger [Z] and the references therein for more details. Our framework of study will be in the mean field regime where the condensate can be described by a Gross Pitaevskii type energy with a term modeling the optical lattice potential. The mean field description of a condensate by the Gross Pitaevskii energy has been derived as the limit of the hamiltonian for N bosons, when N tends to infinity [LSY, LS] in the case of a condensate without optical lattice. The scattering length a_N of the interaction in the N-body problem is such that $Na_N \to g$. The rigorous derivation in the case of an optical lattice where there are fewer atoms per site is nevertheless open. In a one-dimensional optical lattice, the condensate splits into a stack of weakly-coupled disk-shaped condensates, which leads to some intriguing analogues with high-Tc superconductors due to their similar layered structure [SnSt1, SnSt2, KMPS, ABB1, ABB2, ABS]. Our aim, in this paper, is to address mathematical models that describe a BEC in an optical lattice. The theory which we will develop is inspired by a series of physics papers [Sn, SnSt1, SnSt2, KMPS, STKB]. We want to justify their reduction to simpler energy functionals in certain regimes of parameters and in particular understand the ground state energy.

The ground state energy of a rotating Bose-Einstein condensate is given by the minimization of

$$Q_\Omega(\Psi) := \int_{\mathbb{R}^3} \left(\frac{1}{2}|\nabla\Psi - i\Omega \times \mathbf{r}\Psi|^2 - \frac{1}{2}\Omega^2 r^2\, |\Psi|^2 \, + (V(\mathbf{r}) + W_\epsilon(z))|\Psi|^2 + g|\Psi|^4 \right) dxdydz\,, \tag{1.1}$$

under the constraint

$$\int_{\mathbb{R}^3} |\Psi(x,y,z)|^2 \, dxdydz = 1\,, \tag{1.2}$$

where

- $r^2 = x^2 + y^2\,,\ \mathbf{r} = (x,y,z)\,,$
- $\Omega \geq 0$ is the rotational velocity along the z axis,
- $\Omega \times \mathbf{r} = \Omega(-y, x, 0)\,,$
- $g \geq 0$ is the scattering length.

The experimental device leading to the realization of optical lattices requires a trapping potential $V(\mathbf{r})$ given by

$$V(\mathbf{r}) = \frac{1}{2}\left(\omega_\perp^2 r^2 + \omega_z^2 z^2\right), \tag{1.3}$$

corresponding to the magnetic trap. We assume that the radial trapping frequency is much larger than the axial trapping frequency, that is

$$0 \leq \omega_z << \omega_\perp\,. \tag{1.4}$$

We will always assume the condition :

$$0 \leq \Omega < \omega_\perp \tag{1.5}$$

for the existence of a minimizer. The trapping has to be stronger than the centrifugal force. The presence of the one dimensional optical lattice in the z direction is modeled by

$$W_\epsilon(z) = \frac{1}{\epsilon^2}\mathbf{w}(z)\,, \tag{1.6}$$

where $\frac{1}{\epsilon^2}$ is the lattice depth[1], and w is a positive T-periodic function. In the whole paper, we will assume :

Assumption 1.1.
The potential $\mathbf{w}$ *is a* C^∞ *even, non negative function on* $\mathbb{R}$ *which is* T*-periodic and admits as unique minima the points* kT $(k \in \mathbb{Z})$*. Moreover these minima are non degenerate. Thus,*

$$\mathbf{w}(z+T) = \mathbf{w}(z)\,,\ \mathbf{w}(0) = 0\,,\ \mathbf{w}''(0) > 0\,,\ \mathbf{w}(z) > 0 \textit{ if } z \notin T\mathbb{Z}\,. \tag{1.7}$$

An example is

$$\mathbf{w}(z) = \sin^2(\frac{2\pi z}{\lambda}) \tag{1.8}$$

and λ is the wavelength of the laser light. The optical potential W_ϵ creates a one-dimensional lattice of wells separated by a distance $T = \lambda/2$. We will assume that ϵ tends to 0 (this means deep lattice) and that T is fixed. Furthermore, we assume that the lattice is deep enough so that it dominates over the magnetic trapping potential in the z direction and that the number of sites is large. Thus we will, in this paper, ignore the magnetic trap in the z direction, and this will correspond to the case

$$\omega_z = 0\,. \tag{1.9}$$

[1] called V_z in Snoek [Sn]

We will mainly discuss, instead of a problem in $\mathbb{R}^3$, a periodic problem in the z direction, that is in $\mathbb{R}^2_{x,y}\times[-\frac{T}{2},\frac{T}{2}[$, where T corresponds to the period of the optical lattice, or in $\mathbb{R}^2_{x,y}\times[-\frac{NT}{2},\frac{NT}{2}[$ for a fixed integer $N\geq 1$. Therefore, we focus (see however Subsection 8.2 for a justification of this choice) on the minimization of the functional

$$
\begin{aligned}
&Q_\Omega^{per,N}(\Psi):=\\
&\int_{\mathbb{R}^2_{x,y}\times]-\frac{NT}{2},\frac{NT}{2}[}\left(\frac{1}{2}|\nabla\Psi-i\Omega\times\mathbf{r}\Psi|^2-\frac{1}{2}\Omega^2r^2|\Psi|^2+(V(\mathbf{r})+W_\epsilon(z))|\Psi|^2+g|\Psi|^4\right)dxdydz\,,
\end{aligned}
\tag{1.10}
$$

under the constraint

$$
\int_{\mathbb{R}^2_{x,y}\times]-\frac{NT}{2},\frac{NT}{2}[}|\Psi(x,y,z)|^2\,dxdydz=1\,, \tag{1.11}
$$

with

$$
V(\mathbf{r})=\frac{1}{2}{\omega_\perp}^2r^2\,, \tag{1.12}
$$

the potential W_ϵ given by (1.6)-(1.7), and the wave function Ψ satisfying

$$
\Psi(x,y,z+NT)=\Psi(x,y,z)\,. \tag{1.13}
$$

This functional has a minimizer in the unit sphere of its natural form domain (see (8.10) for its description) $\mathcal{S}_\Omega^{per,N}$ and we call

$$
E_\Omega^{per,N}=\inf_{\Psi\in\mathcal{S}_\Omega^{per,N}}Q_\Omega^{per,N}(\Psi)\,. \tag{1.14}
$$

Notation

In the case $N=1$, we will write more simply

$$
Q_\Omega^{per}:=Q_\Omega^{per,(N=1)}\,,\ E_\Omega^{per}:=E_\Omega^{per,(N=1)}\,. \tag{1.15}
$$

When $\Omega=0$, we will sometimes omit the reference to Ω.

Our aim is to justify that the ground state energy can be well approximated by the study of simpler models introduced in physics papers [Sn, SnSt1, KMPS] and to measure the error which is done in the approxiamtion. For that purpose, we will describe how, in certain regimes, the semi-classical analysis developed for linear problems related to the Schrödinger operator with periodic potential or multiple wells potentials is relevant: Outassourt [Ou], Helffer-Sjöstrand [He, DiSj] or for an alternative approach [Si].

1.2 The linear model

The linear model which appears naturally is a selfadjoint realization associated with the differential operator :

$$H_\Omega = H_\perp^\Omega + H_z \,, \tag{1.16}$$

with

$$H_\perp^\Omega := -\frac{1}{2}\Delta_{x,y} + \frac{1}{2}\omega_\perp^2 r^2 - \Omega L_z \,, \tag{1.17}$$

$$L_z = i(x\partial_y - y\partial_x) \,, \tag{1.18}$$

and

$$H_z := -\frac{1}{2}\frac{d^2}{dz^2} + W_\epsilon(z) \,. \tag{1.19}$$

In the transverse direction, we will consider the unique natural selfadjoint extension in $L^2(\mathbb{R}^2_{x,y})$ of the positive operator $H_\perp^\Omega$ by keeping the same notation. In the longitudinal direction, we will consider specific realizations of H_z and in particular the T-periodic problem or more generally the (NT)-periodic problem attached to H_z which will be denoted by H_z^{per} and $H_z^{per,N}$ and we keep the notation H_z for the problem on the whole line.
So our model will be the self-adjoint operator

$$H_\Omega^{per,N} = H_\perp^\Omega + H_z^{per,N} \,. \tag{1.20}$$

In this situation with separate variables, we can split the spectral analysis, the spectrum of $H_\Omega^{per,N}$ being the closed set

$$\sigma(H_\Omega^{per,N}) := \sigma(H_\perp^\Omega) + \sigma(H_z^{per,N}) \,. \tag{1.21}$$

The first operator $H_\perp^\Omega$ is a harmonic oscillator with discrete spectrum as we will explain in Section 2. Under Condition (1.5), the bottom of its spectrum is given by

$$\lambda_1^\perp := \inf(\sigma(H_\perp^\Omega)) = \omega_\perp \,, \tag{1.22}$$

hence is independent of Ω.
A corresponding groundstate is the Gaussian $\psi_\perp = \left(\frac{\omega_\perp}{\pi}\right)^{\frac{1}{2}} \exp -\frac{\omega_\perp}{2} r^2$. The gap between the ground state energy and the second eigenvalue (which has multiplicity 1 or 2) is given by

$$\delta_\perp := \lambda_{2,\Omega}^\perp - \lambda_1^\perp = \omega_\perp - \Omega \,. \tag{1.23}$$

The properties of the periodic Hamiltonian $H_z^{per,N}$, which will be described in Subsection 3.2 (Formulas (3.8) and (3.9) for the physical model), depend on the value of N. In the case $N = 1$, we call the groundstate of H_z^{per} $\phi_1(z)$ and the ground energy (or lowest eigenvalue) $\lambda_{1,z}$. In the semi-classical regime $\epsilon \to 0$, $\lambda_{1,z}$ satisfies

$$\lambda_{1,z} \sim \frac{c}{\epsilon}, \tag{1.24}$$

for some $c > 0$. The splitting δ_z between the groundstate energy and the first excited eigenvalue satisfies

$$\delta_z \sim \frac{\tilde{c}}{\epsilon}, \tag{1.25}$$

for some $\tilde{c} > 0$.
For $N > 1$, the groundstate energy of $H_z^{per,N}$ is unchanged and the corresponding groundstate ϕ_1^N is the periodic extension of ϕ_1 considered as an (NT)-periodic function. More precisely, in order to have the L^2- normalizations, the relation is

$$\phi_1^N = \frac{1}{\sqrt{N}}\phi_1 \,, \tag{1.26}$$

on the line. But we have now N exponentially close eigenvalues of the order of $\lambda_{1,z}$ lying in the first band of the spectrum of H_z on the whole line. They are separated from the $(N+1)$-th by a splitting δ_z^N which satisfies :

$$\delta_z^N = \delta_z + \widetilde{\mathcal{O}}(\exp -S/\epsilon))\,. \tag{1.27}$$

Here the notation $\widetilde{\mathcal{O}}(\exp -S/\epsilon))$ means

$$\widetilde{\mathcal{O}}(\exp -S/\epsilon)) = \mathcal{O}(\exp -S'/\epsilon)\,,\ \forall S' < S\,. \tag{1.28}$$

The first N eigenfunctions satisfy

$$\phi_\ell^N(z+T) = \exp(\frac{2i\pi(\ell-1)}{N})\ \phi_\ell^N(z)\,,\ \ \text{for } \ell = 1,\dots,N\,, \tag{1.29}$$

corresponding to the special values $k = \frac{2\pi(\ell-1)}{NT}$ of what will be called later a k-Floquet condition (see (A.2)).

We will sometimes use another real orthonormal basis (called (NT)-periodic Wannier functions basis) (ψ_j^N) $(j = 0,\dots,N-1)$ of the spectral space attached to the first N eigenvalues. Each of these (NT)-periodic functions have the advantage to be localized (as $\epsilon \to 0$) in a specific well of W_ϵ considered as defined on $\mathbb{R}/(NT)\mathbb{Z}$.

1.3 The reduced functionals

We want to prove the reduction to lower dimensional functionals by using the spectral analysis of the linear problem. There are two natural ideas to compute upper bounds, and thus find these functionals. We can

- either use test functions of the type

$$\Psi(x,y,z) = \phi(z)\psi_\perp(x,y)\,, \tag{1.30}$$

  where $\psi_\perp$ is the first normalized eigenfunction of $H_\perp^\Omega$ and minimize among all possible L^2-normalized $\phi(z)$ to obtain a 1D-longitudinal reduced problem,

- or use

  - in the case $N = 1$,

$$\Psi(x,y,z) = \phi_1(z)\psi(x,y) \tag{1.31}$$

    where ϕ_1 is the first eigenfunction of H_z^{per} and minimize among all possible L^2-normalized $\psi(x,y)$ to obtain a 2D transverse reduced problem,

  - or in the case $N \geq 1$

$$\Psi(x,y,z) = \sum_{j=0}^{N-1} \psi_j^N(z)\psi_{j,\perp}(x,y) \tag{1.32}$$

    where $\psi_j^N(z)$ is the orthonormal basis of Wannier functions mentioned above, and minimize on the suitably normalized $\psi_{j,\perp}$'s which provide N coupled problems. We denote by Π_N the projection on this space. For $\Psi \in L^2(\mathbb{R}^2 \times]-\frac{NT}{2}, \frac{NT}{2}[)$, we have

$$\Pi_N \Psi = \sum_{j=0}^{N-1} \psi_j^N(z)\psi_{j,\perp}(x,y)\,, \tag{1.33}$$

    with

$$\psi_{j,\perp}(x,y) = \int_{]-\frac{NT}{2},\frac{NT}{2}[} \Psi(x,y,z)\psi_j^N(z)\,dz\,.$$

Computing the energy of a test function of type (1.30), we get

$$Q_\Omega^{per,N}(\Psi) = \omega_\perp + \mathcal{E}_A^N(\phi) \tag{1.34}$$

where $\mathcal{E}_A^N$ is the functional on the NT-periodic functions in the z direction, defined on $H^1(\mathbb{R}/NT\mathbb{Z})$ by

$$\phi \mapsto \mathcal{E}_A^N(\phi) = \int_{-\frac{NT}{2}}^{\frac{NT}{2}} \left(\frac{1}{2}|\phi'(z)|^2 + W_\epsilon(z)|\phi(z)|^2 + \widehat{g}\,|\phi(z)|^4\right)\, dz \tag{1.35}$$

with

$$\widehat{g} := g\left(\int_{\mathbb{R}^2} |\psi_\perp(x,y)|^4\, dxdy\right) = \frac{1}{2\pi} g\omega_\perp. \tag{1.36}$$

The functional $\mathcal{E}_A^N$ is introduced by [KMPS] who analyze a particular case. Its study in the small ϵ limit is one of the aims of this paper.

For test functions of type (1.31), we get in the case $N = 1$

$$Q_\Omega^{per}(\Psi) = \lambda_{1,z} + \mathcal{E}_{B,\Omega}(\psi) \tag{1.37}$$

with

$$\begin{aligned}&\mathcal{E}_{B,\Omega}(\psi)\\ &:= \int_{\mathbb{R}^2_{x,y}} \left(\frac{1}{2}|\nabla_{x,y}\psi - i\Omega\times\mathbf{r}\psi|^2 - \frac{1}{2}\Omega^2 r^2|\psi|^2 + \frac{1}{2}\omega_\perp^2(x^2+y^2)|\psi|^2 + \widetilde{g}|\psi|^4\right)\, dx\, dy\,,\end{aligned} \tag{1.38}$$

and

$$\widetilde{g} := g\left(\int_{-\frac{T}{2}}^{\frac{T}{2}} |\phi_1(z)|^4\, dz\right)\,. \tag{1.39}$$

In the case $N > 1$, we define $\mathcal{E}_{B,\Omega}^N((\psi_{j,\perp})_{j=0,\dots,N-1})$ by

$$Q_\Omega^{per,N}(\Psi) := \lambda_{1,z} \sum_j ||\psi_{j,\perp}||^2 + \mathcal{E}_{B,\Omega}^N((\psi_{j,\perp})) \tag{1.40}$$

with

$$\Psi = \sum_{j=0}^{N-1} \psi_j^N(z)\psi_{j,\perp}(x,y)\,. \tag{1.41}$$

Of course when minimizing over normalized Ψ's, one gets more simply the problem of minimizing

$$Q_\Omega^{per,N}(\Psi) = \lambda_{1,z} + \mathcal{E}_{B,\Omega}^N((\psi_{j,\perp}))\,. \tag{1.42}$$

As such, the energy $\mathcal{E}^N_{B,\Omega}$ does not provide N coupled problems but one single energy depending on N test functions. Nevertheless, in the small ϵ limit, the Wannier functions are localized in each well. Thus each function $\psi_{j,\perp}$ only interacts with its nearest neighbors and this simplification provides N coupled problems, as suggested by Snoek [Sn] on the basis of formal computations. We will analyze their validity. This reduced functional is somehow related to the Lawrence-Doniach model for superconductors (see [ABB1, ABB2]).

1.4 Main results

1.4.1 Universal estimates and applications

The analysis of the linear case immediately leads to the following trivial and universal inequalities (which are valid for any N and any Ω such that $0 \leq \Omega < \omega_\perp$)

$$\lambda_{1,z} + \omega_\perp \leq E^{per,N}_\Omega \leq \lambda_{1,z} + \omega_\perp + I_N \,, \tag{1.43}$$

where

$$I_N := \frac{g\omega_\perp}{2N\pi} \left(\int_{-\frac{T}{2}}^{\frac{T}{2}} |\phi_1(z)|^4 dz \right) = \frac{I}{N} \,. \tag{1.44}$$

This universal estimate is obtained by using the test function

$$\Psi^{per,N}(x,y,z) = \psi_\perp(x,y)\phi_1^N(z) \,,$$

where ϕ_1^N is the N-th normalized ground state introduced in (1.26) and $\psi_\perp(x,y)$ is the ground state of $H^\Omega_\perp$, actually independent of Ω.
From (1.26), we have :

$$\int_{-\frac{NT}{2}}^{\frac{NT}{2}} (\phi_1^N(z))^4 \, dz = \frac{1}{N^2} \int_{-\frac{NT}{2}}^{\frac{NT}{2}} \phi_1(z)^4 \, dz = \frac{1}{N} \int_{-\frac{T}{2}}^{\frac{T}{2}} \phi_1(z)^4 \, dz \,, \tag{1.45}$$

where, as $\epsilon \to 0$, and, under Assumption (1.7), it can be proved (see (3.10)) that

$$\int_{-\frac{T}{2}}^{\frac{T}{2}} \phi_1(z)^4 \, dz \sim c_4 \, \epsilon^{-\frac{1}{2}} \,, \tag{1.46}$$

for some explicitly computable constant $c_4 > 0$.
Thus, we have the following estimate for I_N

$$I_N \sim \frac{c_4}{2\pi} \frac{g\omega_\perp}{N} \, \epsilon^{-\frac{1}{2}} \,. \tag{1.47}$$

An immediate analysis shows that $\lambda_{1,z} + \omega_\perp$ is a good asymptotic of $E_\Omega^{per,N}$ in the limit $\epsilon \to 0$ when g is sufficiently small (what we can call the quasi-linear situation). More precisely, we have

Theorem 1.2.
Under the condition that either

$$(QLa) \quad g << \epsilon^{\frac{1}{2}}\,, \tag{1.48}$$

or

$$(QLb) \quad g\omega_\perp \epsilon^{\frac{1}{2}} << 1\,, \tag{1.49}$$

then we have

$$E_\Omega^{per,N} = (\lambda_{1,z} + \omega_\perp)\,(1 + o(1))\,, \tag{1.50}$$

as ϵ tends to 0.

Each of these conditions implies indeed that I_N is small relatively to λ_z or to $\omega_\perp$.

So our goal is

- to have more accurate estimates than (1.50),
- to analyze more interesting cases when none of these two conditions is satisfied and to give natural sufficient conditions allowing the analysis of reduced models.

We are able to justify the reductions to the lower dimensional functionals $\mathcal{E}_A^N$ and $\mathcal{E}_{B,\Omega}^N$ when their infimum is much smaller than the gap between the first two excited states of the linear problem in the other direction, namely in case A, when m_A^N is much smaller than $\delta_\perp$, where

$$m_A^N = \inf_{||\phi||=1} \mathcal{E}_A^N(\phi)\,, \tag{1.51}$$

and in case B, when $m_{B,\Omega}^N$ is much smaller than $1/\epsilon$, the gap between the two first bands of the periodic problem on the line, where

$$m_{B,\Omega}^N = \inf_{\sum_j ||\psi_{j,\perp}||^2=1} \mathcal{E}_{B,\Omega}^N((\psi_{j,\perp}))\,. \tag{1.52}$$

An independent difficulty is then to have more accurate estimates m_A^N and $m_{B,\Omega}^N$ according to the regime of parameters. We do not have universal estimates for this but have to separate two cases :

- the Weak Interaction case, where the interaction term (L^4 term) is at most of the same order as the ground state of the linear problem in the same direction;
- the Thomas Fermi case, where the kinetic energy term is much smaller than the potential and interaction terms.

In what follows, when N is not mentioned in m_A^N, $m_{B,\Omega}^N$, $\mathcal{E}_A^N$, $\mathcal{E}_{B,\Omega}^N$, then the notations are for $N = 1$. Similarly, if Ω is not mentioned, this means that either the considered quantity is independent of Ω or that we are treating the case $\Omega = 0$. To mention the dependence on other parameters, we will sometimes explictly write this dependence like for example $m_A^N(\epsilon, \widehat{g})$ or $m_{B,\Omega}^N(\tilde{g}, \omega_\perp)$.

1.4.2 Case (A) : the longitudinal model

We consider states which are of type (1.30) with $\varphi \in L^2(\mathbb{R}_z/(NT)\mathbb{Z})$. The energy of such test functions provides the upper bound

$$E_\Omega^{per,N} \leq \omega_\perp + m_A^N(\epsilon, \widehat{g}) \tag{1.53}$$

where m_A^N is given by (1.51) and $\widehat{g}$ was introduced in (1.36).

In order to show that the upper bound is an approximate lower bound, we first address the "Weak Interaction" case,

$$(AWIa) \quad 1 << \epsilon(\omega_\perp - \Omega)\,, \tag{1.54}$$

and, for a given $c > 0$,

$$(AWIb) \quad g\omega_\perp \epsilon^{\frac{1}{2}} \leq c\,. \tag{1.55}$$

The first assumption implies that the lowest eigenvalue $\lambda_{1,z}$ of the linear problem in the z direction (having in mind (1.24)) is much smaller than the gap in the transverse direction $\delta_\perp = \omega_\perp - \Omega$. This will allow the projection onto the subspace $\psi_\perp \otimes L^2(\mathbb{R}_z/(NT)\mathbb{Z})$. The second assumption implies that the nonlinear term (of order $g\omega_\perp/\sqrt{\epsilon}$) is of the same order as $\lambda_{1,z}$. It implies using (1.24), (1.47) and the universal estimate

$$\lambda_{1,z} \leq m_A^N \leq \lambda_{1,z} + I_N\,, \tag{1.56}$$

that

$$m_A^N \approx \frac{1}{\epsilon}\,. \tag{1.57}$$

Here $\approx$ means "of the same order" in the considered regime of parameters. More precisely we mean by writing (1.57) that, for any $\epsilon_0 > 0$, there exists $C > 0$ such that, for all $\epsilon \in]0, \epsilon_0]$, any $g, \omega_\perp$ satisfying (1.55),

$$\frac{1}{C\epsilon} \leq m_A^N \leq \frac{C}{\epsilon}\,.$$

Note that most of the time, we will not control the constant with respect to N.

All these rough estimates are obtained by rather elementary semi-classical methods which are recalled in Section 3. More precise asymptotics of m_A^N will be given under the additional Assumption (1.48) in Section 5.2. Thus, by (1.54), m_A^N is much smaller than $\delta_\perp$. We will prove

Theorem 1.3.

When ϵ tends to 0, and under Conditions (1.54) and (1.55), we have

$$E_\Omega^{per,N} = \omega_\perp + m_A^N(\epsilon, \widehat{g})\,(1 + o(1))\,. \tag{1.58}$$

We now describe the "Thomas-Fermi" regime, where we can also justify the reduction to the longitudinal model. We assume that, for some given $c > 0$,

$$(ATFa) \quad g\omega_\perp\sqrt{\epsilon} >> 1\,, \tag{1.59}$$

$$(ATFb) \quad g\omega_\perp\epsilon^2 \leq c\,, \tag{1.60}$$

$$(ATFc) \quad g^{\frac{5}{12}}\epsilon^{-\frac{1}{6}}\omega_\perp{}^{\frac{5}{12}} << (\omega_\perp - \Omega)^{\frac{3}{8}}\,. \tag{1.61}$$

Note that (1.59) is the converse of (1.55) while (1.59) and (1.61) imply that $1 << \epsilon(\omega_\perp - \Omega)$. This implies $\lambda_{1,z} << \delta_\perp$, which is the main condition to reduce to case A. Assumptions (1.59) and (1.60) allow to show that :

$$m_A^N \approx \left(\frac{g\omega_\perp}{\epsilon}\right)^{\frac{2}{3}}\,, \tag{1.62}$$

and this also implies that the nonlinear term is much bigger than δ_z.

The estimate (1.62) will be shown in Section 5.3, together with more precise ones with stronger hypotheses (see Assumption (5.19) and (5.20)).

Theorem 1.4.

When ϵ tends to 0*, and under Conditions* (1.59), (1.60) *and* (1.61)*, we have, as $\epsilon \to 0$,*

$$E_\Omega^{per,N} = \omega_\perp + m_A^N(\epsilon, \widehat{g})\,(1 + o(1))\,. \tag{1.63}$$

The proofs give actually much stronger results.

1.4.3 Case (B) : the transverse model

This corresponds to the idea of a reduction on the ground eigenspace in the z variable, where the interaction term is kept in the transverse problem: therefore, this is a regime where $\omega_\perp \epsilon << 1$. We recall that we denote by $\lambda_{1,z}$ the (N-independent) ground state energy of $H_z^{per,N}$ and by ϕ_1^N the normalized ground state. We consider states which are of type (1.31) or (1.32). We have defined $\mathcal{E}_{B,\Omega}^N$ by (1.40)-(1.41) and $m_{B,\Omega}^N$, the infimum of the energy of such test functions by (1.52). We have the upper bound

$$E_\Omega^{per,N} \leq \lambda_{1,z} + m_{B,\Omega}^N \,. \tag{1.64}$$

When $N = 1$, $m_{B,\Omega}$ is a function of $\tilde{g}$ and $\omega_\perp$ as it is clear from (1.38) and (1.52). Note that, from (1.46), we get

$$\tilde{g} = g(\int_{-\frac{T}{2}}^{\frac{T}{2}} \phi_1(z)^4 dz) \approx \frac{g}{\sqrt{\epsilon}} \,. \tag{1.65}$$

Again we can discuss two different cases according to the size of the interaction. In the Weak Interaction case, we prove the following :

Theorem 1.5.
When ϵ tends to 0, and under the conditions

$$(BWIa) \quad g\epsilon^{-\frac{1}{2}} \leq C \,, \tag{1.66}$$

$$(BWIb) \quad \omega_\perp \epsilon << 1 \,, \tag{1.67}$$

then

$$E_\Omega^{per,N} = \lambda_{1,z} + m_{B,\Omega}^N (1 + o(1)) \,. \tag{1.68}$$

Condition (BWIb) implies that the bottom of the spectrum of the linear problem in the $x - y$ direction is much smaller than δ_z, the gap in the z direction, which is of order $1/\epsilon$. Condition (1.66), together with (1.43) and (1.47), implies that $m_{B,\Omega}^N$ satisfies

$$m_{B,\Omega}^N \approx \omega_\perp \,. \tag{1.69}$$

Indeed, (BWIa) and (BWIb) imply $g\epsilon^{\frac{1}{2}}\omega_\perp << 1$, that is (QLb).

In the Thomas-Fermi case, we prove the following :

Theorem 1.6.
When ϵ tends to 0, and under the conditions

$$(BTFa) \quad \sqrt{\epsilon} << g\,, \tag{1.70}$$

$$(BTFb) \quad \omega_\perp \sqrt{g} \epsilon^{\frac{3}{4}} << 1\,, \tag{1.71}$$

and

$$(BTFc) \quad g^{\frac{3}{2}} \epsilon^{\frac{1}{4}} \omega_\perp << 1\,, \tag{1.72}$$

then

$$E_\Omega^{per,N} = \lambda_{1,z} + m_{B,\Omega}^N (1 + o(1))\,. \tag{1.73}$$

Note that $(BTFa)$ is the converse of $(BWIa)$. We will see in Proposition 6.3 (together with (6.4), (6.16) and (6.49)) that, under these assumptions and Assumption (6.15), the term $m_{B,\Omega}^N$ satisfies

$$m_{B,\Omega}^N \approx \omega_\perp \sqrt{g}/\epsilon^{1/4}\,, \tag{1.74}$$

and thus is much smaller than δ_z^N which is of order $\frac{1}{\epsilon}$.

Our proofs are made up of two parts : rough or accurate estimates of $m_{A,\Omega}^N$ and $m_{B,\Omega}^N$ on the one hand and a lower bound for $E_\Omega^{per,N}$ on the other hand. The lower bound consists in showing that the upperbound obtained by projecting on the special states introduced above in (1.30), (1.31) or (1.32) is actually also asymptotically a good lower bound.

1.4.4 Tunneling effect and discrete model

Since the Wannier functions are localized in the z variable, the energy of a function $\Psi = \sum_{j=0}^{N-1} \psi_j^N(z)\psi_{j,\perp}(x,y)$ provides at leading order the sum of N decoupled energies for $\psi_{j,\perp}$ on each slice j. At the next order, in the computation of the L^2 norm of the gradient, only the nearest neighbors in z interact through an exponentially small term, describing what is called the tunneling effect. These simplifications are discussed in section 7. We are lead to new functionals and in particular a discrete model that we analyze in relationship with the physics papers.

In case A, the behavior on each slice j is the same, given by $\psi_\perp$ and it is the behavior on the z direction which has a tunneling contribution. There are no vortices whatever the velocity Ω.

In case B, for $N = 1$, there are vortices for large velocity and they are located on each slice at the same place. For N large, it is an open and interesting question to analyze whether it is possible for a vortex line to vary location according to the slice, whether vortices interact between the slices and how. This could be performed using our reduced models.

1.5 Organization of the paper

The paper is organized as follows. In Section 2, we start the spectral analysis of the linear problems in the longitudinal and transverse directions. We recall in particular the main techniques which can be used for the analysis of the spectral problem with periodic potential on the line. Section 3 is devoted to the semi-classical results for the periodic problem. Although we are mainly interested in $1D$-problems we recall here techniques which are true in any dimension and can be useful for the analysis of $2D$ or $3D$ optical lattices.

In Section 4, we prove the main theorems for case A. In Section 5, we analyze the ground state of the $1D$ nonlinear energy $\mathcal{E}_A^N$ for $N = 1$ and $N > 1$ and also distinguish between the two cases: Weak Interaction and Thomas-Fermi. Section 6 corresponds to a similar analysis for the transverse models $\mathcal{E}_B^N$. Section 7 is devoted to the tunneling effects and discuss, on the basis of the semi-classical estimates of Section 3, some results by physicists on the discrete nonlinear Schrödinger model. In Section 8, we analyze various boundary conditions and compare in particular the problems on $\mathbb{R}^3$ (which is completely solved) and the problems on $\mathbb{R}^2\times] - \frac{NT}{2}, \frac{NT}{2}[$ with periodic condition which seem physically more interesting.

2 Analysis of the linear model

The linear model which appears naturally is associated to

$$H_\Omega = H_\perp^\Omega + H_z \,,$$

which was presented in the introduction (see (1.17)-(1.21)). A natural condition (for the strict positivity of the operator $H_\perp^\Omega$) is Condition (1.5). In this situation with separate variables, we can split the spectral analysis in the separate spectral analysis of $H_\perp^\Omega$ and the spectral analysis of a suitable realization of H_z which will be presented in the next subsection.

2.1 The harmonic oscillator in the transverse variable

For simplicity, we begin the analysis of $H_\perp = H_\perp^\Omega$ with the case $\Omega = 0$.
The first operator $H_\perp^{\Omega=0}$ is a harmonic oscillator with discrete spectrum and the bottom of its spectrum is given by

$$\inf(\sigma(H_\perp^0)) = \omega_\perp \,. \tag{2.1}$$

A corresponding L^2-normalized ground state is the Gaussian

$$\psi_\perp = \left(\frac{\omega_\perp}{\pi}\right)^{\frac{1}{2}} \exp -\frac{\omega_\perp}{2} r^2 \,. \tag{2.2}$$

Moreover the gap between the ground state energy and the second eigenvalue (which has multiplicity 2) is given by

$$\lambda_{2,\perp} - \omega_\perp = \omega_\perp \,. \tag{2.3}$$

The spectrum of $H_\perp^\Omega$ can be recovered by considering first the joint spectrum of $H_\perp^\Omega$ and L_z. For each eigenspace of L_z corresponding to ℓ for some $\ell \in \mathbb{Z}$, we can look at the operator

$$H_\perp^{(\ell)} := -\frac{1}{2}\Delta_{x,y} + \frac{1}{2}{\omega_\perp}^2 r^2 - \Omega\ell \,, \tag{2.4}$$

considered as an unbounded operator on $L^2(\mathbb{R}^2) \cap \text{ Ker } (L_z - \ell)$.

More precisely, for Ω satisfying (1.5), a common eigenbasis of L_z and $H_\perp^0$ is given by the set of (not normalized) Hermite functions:

$$\phi_{j,k}(x,y) = e^{\frac{\omega_\perp}{2}(x^2+y^2)} \, (\partial_x + i\partial_y)^j \, (\partial_x - i\partial_y)^k \left(e^{-\omega_\perp(x^2+y^2)}\right) \tag{2.5}$$

where j and k are non-negative integers.
The eigenvalues are $(j-k)$ for L_z and

$$E_{j,k} = \omega_\perp + (\omega_\perp - \Omega)j + (\omega_\perp + \Omega)k \tag{2.6}$$

for $H_\perp^\Omega$.

The spectrum of $H_\perp^{(\ell)}$ is obtained by considering the pairs (j,k) such that $j - k = \ell$.
We emphasize that this orthogonal basis of eigenfunctions is independent of Ω.

2.2 The band spectrum in the longitudinal direction

The second operator H_z can be analyzed by semi-classical methods but note that our semi-classical parameter is ϵ. One can of course in the case of the specific w introduced in (1.7) recognize this operator as the Mathieu operator (for which a lot of information can be obtained using special functions (see [AS])) but we prefer to give the presentation of the theory for a more general periodic potential w. We hope that the general ideas which are behind will become clearer.

There are two related approaches for the analysis of the spectrum of H_z, which is known to be a band spectrum, i.e. an absolutely continuous spectrum which is a union of closed intervals, which are called the bands.

2.2.1 Floquet's theory

We can first use the Floquet theory (or the Bloch theory, which is an alternative name for the same theory). This is more detailed in the appendix. One can show that the spectrum of H_z is obtained by taking the closure of $\cup_{k\in[0,2\pi/T]}\sigma(H_{z,k})$ where

$$H_{z,k} = -\frac{1}{2}\left(\frac{d}{dz}+ik\right)^2 + W_\epsilon(z)$$

is considered as an operator on $L^2(\mathbb{R}/T\mathbb{Z})$. So

$$\sigma(H_z) = \overline{\cup_{k\in[0,\frac{2\pi}{T}]}\sigma(H_{z,k})}\,. \tag{2.7}$$

We now write

$$\Gamma = T\mathbb{Z} \text{ and } \Gamma^* = \frac{2\pi}{T}\mathbb{Z}\,. \tag{2.8}$$

Hence we have to analyze for each k the operator $H_{z,k}$ on $L^2(\mathbb{R}/\Gamma)$. Later we will use the notation

$$H_z^{per} = H_{z,0}\,. \tag{2.9}$$

A unitary equivalent presentation of this approach consists in analyzing H_z restricted to the subspace $\mathfrak{h}_k$ of the $u\in L^2_{loc}(\mathbb{R})$ such that

$$u(z+T) = e^{ikT}\,u(z)\,. \tag{2.10}$$

Here we did not see a k-dependence in the differential operator but this is the choice of the space $\mathfrak{h}_k$ (which is NOT in $L^2(\mathbb{R})$), which gives the k-dependence. Condition (2.10) is called a Floquet condition.

This means that we have written, using the language of the Hilbertian-integrals, the decomposition

$$L^2(\mathbb{R}) = \int_{[0,2\pi/T]}^{\oplus} \mathfrak{h}_k \, dk \tag{2.11}$$

and that we have for the operator the corresponding decomposition

$$H_z = \int_{[0,2\pi/T]}^{\oplus} \widetilde{H}_{z,k} \, dk \,, \tag{2.12}$$

with $\widetilde{H}_{z,k}$ unitary equivalent to $H_{z,k}$.

For each $k \in [0, 2\pi/T[$, $H_{z,k}$ has a discrete spectrum which can be described by an increasing sequence of eigenvalues $(\lambda_j(k))_{j\in\mathbb{N}}$. The spectrum of H_z is then a union of bands B_j, each band being described by the range of λ_j. At least when we have the additional symmetry W_ϵ even, one can determine for which value of k the ends of the band B_j are obtained. For $j = 1$, we know in addition from the diamagnetic inequality that the minimum of λ_1 is obtained for $k = 0$:

$$\inf_k \lambda_1(k) = \lambda_1(0) \,. \tag{2.13}$$

2.2.2 Wannier's approach

When the band is simple (and this will be the case for the lowest band in the regime ϵ small), one can associate to $\lambda_j(k)$ a normalized[2] eigenfunction $\varphi_j(z,k)$ with in addition an analyticity with respect to k together with the $(2\pi/T)$-periodicity in k.

In this case (we now take $j = 1$), one can associate to φ_1, which satisfies,

$$\varphi_1(z + T; k) = \varphi_1(z, k) \,, \tag{2.14}$$

and

$$\varphi_1(z; k + \frac{2\pi}{T}) = \varphi_1(z, k) \,, \tag{2.15}$$

a family of Wannier's functions $(\psi_\ell)_{\ell\in\Gamma}$ defined by

$$\psi_0(z) = \frac{T}{2\pi} \int_0^{\frac{2\pi}{T}} \exp(ikz) \; \varphi_1(z,k) \, dk \,, \; \psi_\ell(z) = \psi_0(z - \ell) \,, \tag{2.16}$$

[2] in $L^2(] - \frac{T}{2}, \frac{T}{2}[)$,

for $\ell \in \Gamma$.
In addition, we can take ψ_0 real. One can indeed construct φ_1 satisfying in addition the condition

$$\overline{\varphi_1(z,k)} = \varphi_1(z,-k)\,. \tag{2.17}$$

One obtains (after some normalization of ψ_0) that

Proposition 2.1.

(i) The family $(\psi_\ell)_{\ell\in\Gamma}$ gives an orthonormal basis of the spectral space attached to the first band.

(ii) ψ_0 is an exponentially decreasing function.

The second point can be proved using the analyticity[3] with respect to k. This orthonormal basis corresponding to the first band plays the role of the basis $P_j(z)\exp -\frac{|z^2|}{2}$ in the Lowest Landau Level approximation.
Note that we recover $\varphi_1(z,k)$ by the formula

$$\varphi_1(z,k) = \exp(-ikz)\sum_{\ell\in\Gamma}\exp(ik\ell)\;\psi_\ell(z)\,. \tag{2.18}$$

Moreover, the operator A on $\ell^2(\Gamma)$ whose matrix is given by

$$A_{\ell\ell'} = \langle H_z\psi_\ell, \psi_{\ell'}\rangle \tag{2.19}$$

is unitary equivalent to the restriction of H_z to the spectral space attached to the first band.
One can of course observe that A commutes with the translation on $\ell^2(\Gamma)$, so it is a convolution operator by a sequence $a \in \ell^1(\Gamma)$ (actually in the space of the rapidly decreasing sequences $\mathcal{S}(\Gamma)$),

$$A_{\ell\ell'} = a(\ell-\ell')\,, \tag{2.20}$$

which is actually the Fourier series of $k \mapsto \lambda_1(k)$

$$\widehat{\lambda}_1 = a\,, \tag{2.21}$$

where

$$\widehat{\lambda}_1(\ell) := \frac{T}{2\pi}\int_0^{2\pi/T}\exp(-i\ell k)\;\lambda_1(k)\;dk\,. \tag{2.22}$$

So we have

$$(Au)(\ell) = \sum_{\ell'\in\Gamma} a(\ell-\ell')u(\ell')\,,\ \text{for } u\in\ell^2(\Gamma)\,.$$

[3]One can make a contour deformation in the integral defining ψ_0 in (2.16).

2.2.3 (NT)-periodic problem

There is another way to proceed at least heuristically. We keep w T-periodic but look at the (NT)-periodic problem and we analyze this problem. The spectrum is discrete but the idea is that we will recover the band spectrum in the limit $N \to +\infty$. If we compare with what we do in the Floquet theory, the analysis of the (NT)-periodic problem consists in considering the direct sum of the problems with a Floquet condition corresponding to $k = 0, \frac{2\pi}{NT}, \cdots, \frac{2\pi(N-1)}{NT}$.

Note that this decomposition into a direct sum works only for linear problems, so it will be interesting to explore this approach for the non linear problem.

In this spirit, it can be useful to have an adapted orthonormal basis of the spectral space attached to the first N eigenvalues of the NT-periodic problem (which can be identified with the vector space generated by the eigenfunctions corresponding to the N Floquet eigenvalues associated with $k = 0, \frac{2\pi}{NT}, \cdots, \frac{2\pi(N-1)}{NT}$.

Our claim is that there exists an orthonormal basis, for the L^2-norm on $]-\frac{NT}{2}, \frac{NT}{2}[$, consisting of (NT)-periodic functions and replacing the Wannier functions.

We write

$$\psi_0^N(z) = \frac{1}{\sqrt{N}} \sum_{j=1}^{N} \phi_j^N(z)\,, \tag{2.23}$$

where ϕ_j^N is an eigenfunction[4] of the (NT)-periodic problem, chosen in such a way that

$$\phi_j^N(z+T) = \omega_N^{j-1} \phi_j^N(z)\,, \tag{2.24}$$

with $\omega_N = \exp(2i\pi/N)$.
We can then introduce

$$\Gamma^N = \Gamma/(NT\mathbb{Z})\,, \tag{2.25}$$

and define, for $\ell \in \Gamma^N = \Gamma$, the (NT)-Wannier functions

$$\psi_\ell^N(z) = \psi_0^N(z-\ell) \tag{2.26}$$

[4]Note that except in the case $j = 1$, we do not claim that ϕ_j^N is the j-th eigenfunction but this is the first one corresponding to the condition (2.24).

This gives an orthonormal basis of the eigenspace attached to the first N eigenvalues of the (NT)-periodic problem. These first N eigenvalues belong to the previously defined first band.

Note that conversely, we can recover the eigenfunctions ϕ_j^N from the ψ_j^N by a discrete Fourier transfrom. In particular we have

$$\phi_1^N = \frac{1}{\sqrt{N}} \sum_{j=0}^{N-1} \psi_j^N \, . \tag{2.27}$$

Except the fact that these "Wannier" functions are NOT exponentially decreasing at ∞ (they are by construction (NT)-periodic), one can then play with them in the same way (this corresponds to the replacement of the Fourier series by the finite dimensional one). We then meet the "discrete convolution" on $\ell^2(\Gamma^N)$:

$$(A^N u)(\ell) = \sum_{\ell' \in \Gamma^N} a_N(\ell - \ell') u(\ell') \, , \text{ for } u \in \ell^2(\Gamma^N) \, .$$

Of course $\ell^2(\Gamma^N)$ is nothing else than $\mathbb{C}^N$ with its natural Hermitian structure.

We have presented different techniques to determine the bottom of the spectrum of H_z, which all provide the same ground energy. We will now recall more quantitative results based on the so-called semi-classical analysis.

3 Semi-classical analysis for the T-periodic case

3.1 Preliminary discussion

Till now, we have not strongly used that we are in a semi-classical regime: our semi-classical parameter here will not be the Planck constant $\hbar$ (which was already assumed to be equal to 1) but ϵ. We will now use this additional assumption for extracting quantitative results from the previously presented qualitative theory. As already said, the physics literature is analyzing a very particular model, the Mathieu equation. We will rapidly sketch how one can do this in full generality. For the one dimensional case which is considered

here, one can probably refer to Harrell [Ha] (who uses techniques of ordinary differential equations) or to the book of Eastham [Eas], but we will describe a proof which is more general in spirit, which is not limited to the one dimensional situation (see Simon [Si], Helffer-Sjöstrand [HeSj1], Outassourt [Ou]) and is described in the books of Helffer [He] or Dimassi-Sjöstrand [DiSj].
As we have shown in the previous section, the good description of the first band, can be either obtained by a good approximation of $\lambda_1(k)$ and $\varphi_1(z,k)$ as $\epsilon \to 0$ or by first finding a good approximation of the Wannier function ψ_0 introduced in (2.16), which is expected to be exponentially localized in one well, or of the (NT)-periodic Wannier function introduced in (2.23).

The analysis is done usually in two steps. First we localize roughly $\lambda_1(k)$, then we analyze very accurately the variation of $\lambda_1(k) - \lambda_1(0)$.
The first one will be obtained by a harmonic approximation and the second one by the analysis of the tunneling effect.

3.2 The harmonic approximation

We will provide the explanation in a general case containing the model considered by Snoek [Sn] as a particular case. We recall that we work under Assumption 1.1. The statements below are sometimes written vaguely and we refer to [DiSj] or [He] for more precise mathematical statements.
For the approximation of $\lambda_{1,z}(0)$ (actually for any $\lambda_{1,z}(k)$) the rule is that we replace $\mathbf{w}(z)$ (having in mind (1.7)) by its quadratic approximation at 0. The harmonic approximation consists in first looking at the operator

$$-\frac{1}{2}\frac{d^2}{dz^2} + \frac{\mathbf{w}''(0)}{2\epsilon^2} z^2\,, \tag{3.1}$$

on $\mathbb{R}$.
For the model in [Sn], $\mathbf{w}(z) = \sin^2(\frac{\pi z}{T})$, and we find

$$-\frac{1}{2}\frac{d^2}{dz^2} + \frac{1}{\epsilon^2}(\frac{\pi z}{T})^2\,. \tag{3.2}$$

This operator is a harmonic oscillator whose spectrum is explicitly known. The j-th eigenvalue is given by

$$\lambda_{j,z}^{har} = \frac{j-\frac{1}{2}}{\epsilon}\sqrt{\mathbf{w}''(0)}\,. \tag{3.3}$$

The two main pieces of information we have to keep in mind are that the ground state energy is

$$\lambda_{1,z}^{har} = \frac{1}{2\epsilon}\sqrt{\mathbf{w}''(0)}\,, \tag{3.4}$$

and that the gap between the first eigenvalue and the second value is given by

$$\delta_z^{har} := \lambda_{2,z}^{har} - \lambda_{1,z}^{har} = \frac{1}{\epsilon}\sqrt{\mathbf{w}''(0)}\,. \tag{3.5}$$

The corresponding positive L^2 normalized ground state is then given by

$$\psi^{har}(z) = \pi^{-\frac{1}{4}}\mathbf{w}''(0)^{\frac{1}{8}}\,\epsilon^{-\frac{1}{4}}\exp -\mathbf{w}''(0)^{\frac{1}{2}}\frac{z^2}{2\epsilon}\,. \tag{3.6}$$

It will also be important later to have the computation of the L^4 norm. So we get by immediate computation :

$$\int_{\mathbb{R}} \psi^{har}(z)^4\,dz = \pi^{-\frac{1}{2}}\mathbf{w}''(0)^{\frac{1}{4}}\,\epsilon^{-\frac{1}{2}}\,. \tag{3.7}$$

The mathematical result is that this value provides a good approximation of $\lambda_{1,z}(0)$ (and hence of the bottom of the spectrum of H_z) with an error which is $\mathcal{O}(1)$ as $\epsilon \to 0$:

$$\lambda_{1,z}(0) = \lambda_{1,z}^{har} + \mathcal{O}(1)\,. \tag{3.8}$$

By working a little more, one can actually obtain a complete expansion of $\epsilon\lambda_{1,z}(0)$ in powers of ϵ and hence, of $\epsilon\lambda_{1,z}(k)$, since they have the same expansion. For each $j \in \mathbb{N}^*$, one has a similar expansion for $\epsilon\lambda_{j,z}(0)$. This implies in particular an estimate of $\lambda_{2,z}(0) - \lambda_{1,z}(0)$, called the longitudinal gap :

$$\delta_z := \lambda_{2,z}(0) - \lambda_{1,z}(0) = \frac{\sqrt{\mathbf{w}''(0)}}{\epsilon} + \mathcal{O}(1)\ . \tag{3.9}$$

From now on, we simply write $\lambda_{1,z}$ or λ_1 instead of $\lambda_{1,z}(0)$ for the ground state energy of the periodic problem.
Let us note that the ground state of the harmonic oscillator also provides a good approximation of the ground state of H_z^{per}. So we obtain, using (3.7) that for ϕ_1, the L^2-normalized ground state of H_z^{per}, we have

$$\int_{-\frac{T}{2}}^{+\frac{T}{2}} \phi_1(z)^4 dz = \pi^{-\frac{1}{2}}\mathbf{w}''(0)^{\frac{1}{4}}\,\epsilon^{-\frac{1}{2}} + \mathcal{O}(1)\,. \tag{3.10}$$

3.3 The tunneling effect

We now briefly explain the results about the length of the first band, which is exponentially small as $\epsilon \to 0$. The results can take the following form (see the work of Outassourt [Ou] or the book by Dimassi-Sjöstrand, Formula (6.26))

$$\lambda_1(k) - \lambda_1(0) = 2(1 - \cos(kT))\tau + \mathcal{O}(\exp -\frac{S+\alpha}{\epsilon}) \tag{3.11}$$

with $\alpha > 0$ (arbitrarily close from below to 1) and, for some $c_\tau \neq 0$,

$$\tau \sim c_\tau \, \epsilon^{-\frac{3}{2}} \, \exp -\frac{S}{\epsilon} \, . \tag{3.12}$$

Moreover one can express the constants c_τ and S once $\mathbf{w}$ is given (see[5] also [He] in addition to the previous references). This τ seems to be called in some physical literature the hopping amplitude.
Here, we simply explain how one computes S which determines the exponential decay of τ as $\epsilon \to 0$. In any dimension, S is interpreted as the minimal Agmon distance between two different minima of the potential w. In one dimension, with w satisfying Assumption (1.1), this distance is simply the Agmon distance between two consecutive minima and is given by

$$S := \sqrt{2} \int_{-\frac{T}{2}}^{\frac{T}{2}} \sqrt{\mathbf{w}(z)} \, dz \, . \tag{3.13}$$

In particular, when $\mathbf{w}(z) = \sin^2(\frac{\pi z}{T})$, we get

$$S := \sqrt{2} \int_{-\frac{T}{2}}^{\frac{T}{2}} |\sin(\frac{\pi z}{T})| \, dz = \frac{2\sqrt{2}T}{\pi} \, . \tag{3.14}$$

This is to compare to (14) in [SnSt1], which is not an exact formula (as wrongly claimed) but only an asymptotically correct formula. It can be found, for this Mathieu operator, in [AS].
Let us give the formula for the constant c_τ. It can be found in [Ha], see also [Ou], Formula (4.14) and [He] p. 58-59. We have :

$$c_\tau = 2^{\frac{3}{4}} \pi^{-\frac{1}{2}} \exp A_\tau \, , \tag{3.15}$$

with (assuming w even)

$$A_\tau = \lim_{\eta \to 0} \left(\int_\eta^{\frac{T}{2}} \frac{1}{\sqrt{\mathbf{w}(z)}} \, dz + \frac{\sqrt{2}}{\sqrt{\mathbf{w}''(0)}} \ln \eta \right) \, . \tag{3.16}$$

[5] The computation is a little simpler in the case when $\mathbf{w}$ is even.

We just sketch the mathematical proof. Filling out all the wells suitably except one (say 0), we get a new potential $w^{mod} \geq \mathbf{w}$ which coincides with $\mathbf{w}$ in an interval containing 0 and excluding small neighborhoods of all the other minima. We consider, for ϵ small enough, the ground state of this modified problem and (multiplying by a cut-off function) we get a function ψ_0^{app} (and an eigenvalue λ_1^{app}) which is a very good approximation of ψ_0.
Now the hopping amplitude in the abstract theory is given[6] **exactly** by

$$-\tau = a(T) = \langle H_z\psi_0\,,\ \psi_1\rangle = \langle (H_z-\mu)\psi_0\,,\ \psi_1\rangle\,, \tag{3.17}$$

the last equality being satisfied, due to the orthogonality of ψ_0 and ψ_1, for any μ. When replacing ψ_0 by its approximation, one has to be careful, because ψ_0^{app} and $\psi_1^{app} := \psi_0^{app}(\cdot - T)$ are no more orthogonal. So this leads to take $\mu = \lambda_1^{app}$, and one can prove that

$$\tau \sim -\langle (H_z - \lambda_1^{app})\psi_0^{app}\,,\ \psi_1^{app}\rangle\,. \tag{3.18}$$

An easy way to see that τ is exponentially small is to observe that

$$\langle (H_z - \lambda_1^{app})\psi_0^{app}\,,\ \psi_1^{app}\rangle = \epsilon^{-2}\,\langle (\mathbf{w}(z) - w^{mod})\psi_0^{app}\,,\ \psi_1^{app}\rangle\,, \tag{3.19}$$

and to use the information on the asymptotic decay of ψ_0^{app}. The WKB-approximation of ψ_0^{app} is, in a neighborhood of 0,

$$\psi_0^{wkb} = \epsilon^{-\frac14}\, b(z,\epsilon)\exp -\frac{1}{\epsilon}\int_0^z \sqrt{\mathbf{w}(s)}ds\,,\ \text{ for } z \geq 0\,, \tag{3.20}$$

with

$$b(z,\epsilon) \sim \sum_{j\geq 0} b_j(z)\epsilon^j\,, \tag{3.21}$$

and

$$b_0(z) = \pi^{-\frac14}\exp\left(-\int_0^z \frac{(w^{\frac12})'(t) - \sqrt{\frac{\mathbf{w}''(0)}{2}}}{2\sqrt{\mathbf{w}(t)}}\,dt\right)\,. \tag{3.22}$$

It should then be completed by symmetry to get an even WKB solution on $]-T,+T[$.
Note that we have

$$(w^{\frac12})'(T_-) = -\sqrt{\frac{\mathbf{w}''(0)}{2}}\,,$$

which implies that b_0 tends to $+\infty$ as $z \to T_-$.

[6] For the Mathieu potential, this is consistent with Formula (13) in [SnSt1].

An integration by parts together with a WKB approximation leads to the asymptotic estimate of τ announced in (3.12). More precisely, we get that the prefactor c_τ is immediately related to the constant $b_0(\frac{T}{2})^2\sqrt{V(\frac{T}{2})}$ and this leads to (3.15). Note that more generally we have

$$b_0(z)b_0(T-z)\sqrt{V(z)} = \text{ Cst}\,, \tag{3.23}$$

which again shows the blowing up of b_0 at T.

Finally, we emphasize that ψ_0^{wkb} is a good approximation of ψ_0 only in intervals $]-T+\eta, T-\eta[$ for some $\eta > 0$.

One can also see that $a(kT)$ is of the order of $|a(T)|^{|k|}$ (for $k \geq 2$)

$$a(kT) = \widetilde{\mathcal{O}}(\tau^2)\,, \tag{3.24}$$

so it is legitimate in order to compute the width of the first band to forget all the $a(\ell)$ for $\ell \in \Gamma, \ell \neq 0, \pm T$.
Thus, in the k variable, the spectrum (corresponding to the first band) is up to a very small error, of the order of the square of $a(T)$, given by the operator of multiplication in $L^2(\mathbb{R}/\Gamma)$ by the function $a(0) + 2a(T)\cos(kT)$.

Remark 3.1.
What is written above corresponds to the use of Wannier functions on $\mathbb{R}$. One can write a close theory using the (NT)-periodic Wannier functions without modifying the main terms of the asymptotics. In particular, ψ_0^{wkb} is also a good approximation of ψ_0^N in intervals $]-T+\eta, T-\eta[$ for some $\eta > 0$.
The interest of the Wannier functions on $\mathbb{R}$ is that they allow to recover the information for all Floquet eigenvalues (see the discussion in Section 7.1).

4 Justification of the reduction to the longitudinal energy $\mathcal{E}_A^N$

4.1 Main result

In this section, we address the reduction to the energy $\mathcal{E}_A^N$ defined in (1.35) and prove the following theorem (recall that m_A^N is defined in (1.51)):

Theorem 4.1. *If*

$$(A\Omega a) \quad m_A^N(\epsilon, \widehat{g})(\omega_\perp - \Omega)^{-1} << 1 \tag{4.1}$$

and

$$(A\Omega b) \quad g(2\omega_\perp - \Omega) m_A^N(\epsilon, \widehat{g})(\omega_\perp - \Omega)^{-\frac{3}{2}} << 1, \tag{4.2}$$

we have

$$\inf_{||\Psi||=1} \mathcal{E}_\Omega^{per,N}(\Psi) = \omega_\perp + m_A^N(\epsilon, \widehat{g})(1 + o(1)). \tag{4.3}$$

Both Theorem 1.3 and Theorem 1.4 are a consequence of Theorem 4.1 as soon as we have the appropriate rough estimates on m_A^N already presented in the introduction. This is what we explain first in Subsection 4.2 before proving the theorem in Subsection 4.3.

4.2 Proof of Theorem 1.3 and Theorem 1.4

4.2.1 Weak Interaction case

In the Weak Interaction case, we recall from (1.57), that, when (1.55) is satisfied, then

$$m_A^N \approx 1/\epsilon\,. \tag{4.4}$$

Therefore, when (1.54) and (1.55) are satisfied, then (4.1) and (4.2) automatically hold with the observation that

$$g(2\omega_\perp - \Omega)(\omega_\perp - \Omega)^{-\frac{3}{2}} m_A^N(\epsilon, \widehat{g}) \leq C g(2\omega_\perp - \Omega)\epsilon^{\frac{1}{2}}((\omega_\perp - \Omega)\epsilon)^{-\frac{3}{2}} << 1\,,$$

and Theorem 1.3 follows from Theorem 4.1.

4.2.2 Thomas-Fermi case

In the Thomas-Fermi case, we will prove in (5.18) that, when (1.59) and (1.60) are satisfied, then

$$m_A^N \approx (g\omega_\perp/\epsilon)^{2/3}\,. \tag{4.5}$$

Let us verify that, if (1.59), (1.60) and (1.61) are satisfied, then (4.1) and (4.2) hold. This will prove Theorem 1.4.

We get (4.1) in the following way. First we have :

$$(\omega_\perp - \Omega)^{-1} m_A^N(\epsilon, \widehat{g}) \leq C(\omega_\perp - \Omega)^{-1} {\omega_\perp}^{\frac{2}{3}} g^{\frac{2}{3}} \epsilon^{-\frac{2}{3}}\,.$$

Hence (4.1) is a consequence of

$$g\omega_\perp << \epsilon(\omega_\perp - \Omega)^{\frac{3}{2}}\,, \tag{4.6}$$

which follows from (1.61) since (1.59) and (1.61) imply that $(\omega_\perp - \Omega)\epsilon >> 1$. The check of (4.2) is then immediate from (1.61) and (4.5).

4.3 Proof of Theorem 4.1

Because of the upper bound (1.53), Theorem 4.1 is a consequence of the following proposition, recalling that $\delta_\perp = \omega_\perp - \Omega$.

Proposition 4.2.
There exists a constant $C > 0$ such that, for all $\epsilon \in]0,1]$, for all $\omega_\perp$, Ω s.t. $\delta_\perp \geq 1$ and for all $g \geq 0$,

$$\inf_{||\Psi||=1} Q_\Omega^{per,N}(\Psi) = \omega_\perp + m_A^N(\epsilon, \widehat{g})\left(1 - C r_A(\epsilon, \widehat{g})\right)\,, \tag{4.7}$$

with

$$0 \leq r_A(\epsilon, \widehat{g}) \leq g^{1/4} \delta_\perp^{-\frac{1}{8}} \left(\frac{\delta_\perp + \omega_\perp}{\delta_\perp}\right)^{\frac{1}{4}} m_A^N(\epsilon, \widehat{g})^{\frac{1}{4}} + m_A(\epsilon, \widehat{g}) {\delta_\perp}^{-1}\,. \tag{4.8}$$

Proof of the proposition
For simplicity, we make the proof for $\Omega = 0$. Note also that

$$1 - C r_A(\epsilon, \widehat{g}) \geq 0$$

by the lower bound. So we have only to prove (4.8) under the additional condition that the right hand side of (4.8) is less than some fixed α_0 . In any case, the estimate is only interesting in this case !
The proof does not depend on N and for Ω not zero, we will make a remark at the end on how to adapt it, using the diamagnetic inequality.

The proof is inspired by [AB] where a reduction is made from a 3D to a 2D setting for a fast rotation. We project a minimizer Ψ onto $\psi_\perp \otimes L^2(\mathbb{R}/NT\mathbb{Z})$, and call $\psi_\perp(x,y)\,\xi(z)$ its projection:

$$\Psi(x,y,z) = \psi_\perp(x,y)\xi(z) + w(x,y,z) \text{ with } \int_{\mathbb{R}^2} \psi_\perp(x,y) w(x,y,z)\, dxdy = 0\,. \tag{4.9}$$

The orthogonality condition implies in particular

$$1 = \int_{-\frac{NT}{2}}^{\frac{NT}{2}} |\xi(z)|^2\, dz \; + \; \int_{\mathbb{R}^2\times]-\frac{NT}{2},\frac{NT}{2}[} |w(x,y,z)|^2\, dxdydz \tag{4.10}$$

and we have the lower bound

$$\int_{-\frac{NT}{2}}^{\frac{NT}{2}} \mathcal{E}'_B(w(\cdot,\cdot,z))\; dz \ge (\delta_\perp + \omega_\perp) \int_{\mathbb{R}^2\times]-\frac{NT}{2},\frac{NT}{2}[} |w(x,y,z)|^2\; dxdydz\,, \tag{4.11}$$

with

$$\mathcal{E}'_B(\psi) = \int_{\mathbb{R}^2} \left(\frac{1}{2} |\nabla_{x,y} \psi(x,y)|^2 + \frac{{\omega_\perp}^2}{2} (x^2+y^2)\, |\psi(x,y)|^2 \right) dxdy\,.$$

We compute the energy of Ψ and use the orthogonality condition and the equation satisfied by $\psi_\perp$ to find that all the cross terms disappear so that

$$\begin{aligned} Q^{N,per}(\Psi) = \omega_\perp & \int_{-\frac{NT}{2}}^{\frac{NT}{2}} |\xi(z)|^2\, dz \; + \; {\mathcal{E}_A^N}'(\xi) \\ & + \int_{\mathbb{R}^2} {\mathcal{E}_A^N}'(w(x,y,\cdot))\; dxdy + \int_{-\frac{NT}{2}}^{\frac{NT}{2}} \mathcal{E}'_B(w(\cdot,\cdot,z))\; dz \\ & \qquad + g \int_{\mathbb{R}^2\times]-\frac{NT}{2},\frac{NT}{2}[} |\Psi(x,y,z)|^4\, dxdydz\,, \end{aligned} \tag{4.12}$$

where

$${\mathcal{E}_A^N}'(\phi) = \int_{-\frac{NT}{2}}^{\frac{NT}{2}} \left(\frac{1}{2} |\phi'(z)|^2 + W_\epsilon(z) |\phi|^2 \right) dz\,.$$

From (4.10), (4.11) and (4.12), we find

$$Q^{N,per}(\Psi) \ge \omega_\perp + \frac{\delta_\perp}{\delta_\perp + \omega_\perp} \int_{-\frac{NT}{2}}^{\frac{NT}{2}} \mathcal{E}'_B(w(\cdot,\cdot,z))\; dz + \int_{\mathbb{R}^2} {\mathcal{E}_A^N}'(w(x,y,\cdot))\; dxdy\,. \tag{4.13}$$

We use (4.13) together with the upper bound (1.53) and (4.11) to derive that

$$\int_{\mathbb{R}^2\times]-\frac{NT}{2},\frac{NT}{2}[} |w(x,y,z)|^2\, dxdydz \le \frac{m_A^N(\epsilon,\widehat{g})}{\delta_\perp}\,. \tag{4.14}$$

Note that the righthand side in (4.14) is very small according to Conditions (4.1) and (4.2).
Note that (4.14) implies

$$\int_{-\frac{NT}{2}}^{\frac{NT}{2}} |\xi(z)|^2 dz \geq 1 - \frac{m_A^N(\epsilon,\widehat{g})}{\delta_\perp}\,. \tag{4.15}$$

Then, we get also,

$$\begin{array}{l} \int_{\mathbb{R}^2\times]-\frac{NT}{2},\frac{NT}{2}[} |\nabla_{x,y} w(x,y,z)|^2\, dxdydz \leq 2\frac{\delta_\perp+\omega_\perp}{\delta_\perp}\;\frac{m_A^N(\epsilon,\widehat{g})}{\omega_\perp}, \\ \int_{\mathbb{R}^2\times]-\frac{NT}{2},\frac{NT}{2}[} |\partial_z w(x,y,z)|^2\, dxdydz \leq 2\; m_A^N(\epsilon,\widehat{g})\,. \end{array} \tag{4.16}$$

The proof of the Sobolev embedding of $H^1(\mathbb{R}^3)$ in $L^6(\mathbb{R}^3)$ gives (see for example [Bre], p. 164, line -1) for a general function v in $H^1(\mathbb{R}^3)$

$$\|v\|_6 \leq 4\|\partial_x v\|_2^{1/3}\|\partial_y v\|_2^{1/3}\|\partial_z v\|_2^{1/3}. \tag{4.17}$$

Here $\|\;\cdot\|_p$ denotes the norm in $L^p(\mathbb{R}^3)$.
In our case, we are working in $H^1(\mathbb{R}^2_{x,y}\times(\mathbb{R}_z/NT\mathbb{Z}))$. A partition of unity in the z variable allows us to extend this estimate also this case, and we get, for another universal constant C,

$$\|w\|_6 \leq C_N\|\partial_x w\|_2^{1/3}\|\partial_y w\|_2^{1/3}\left(\|\partial_z w\|_2^2 + ||w||_2^2\right)^{1/6}\,, \tag{4.18}$$

where this time $||\;\cdot\;||_p$ denotes the norm in $L^p(\mathbb{R}^2_{x,y}\times]-\frac{NT}{2},\frac{NT}{2}[)$.
So we obtain :

$$\|w\|_6 \leq \tilde{C} m_A^N(\epsilon,\widehat{g})^{\frac{1}{2}}\left(\frac{\delta_\perp+\omega_\perp}{\delta_\perp}\right)^{\frac{1}{3}}\,. \tag{4.19}$$

(C, $\tilde{C}$ are N-dependent constants possibly changing from line to line.)
Since by Hölder's Inequality,

$$\|w\|_4 \leq \|w\|_2^{1/4}\|w\|_6^{3/4}\,,$$

we deduce that

$$\|w\|_4 \leq C\; m_A(\epsilon,\widehat{g})^{\frac{1}{2}}{\delta_\perp}^{-\frac{1}{8}}\left(\frac{\delta_\perp+\omega_\perp}{\delta_\perp}\right)^{\frac{1}{4}}\,. \tag{4.20}$$

We expand

$$|\Psi|^4 = |\psi_\perp|^4|\xi|^4 + 2|\psi_\perp|^2|\xi|^2|w|^2 + 4(\Re(\psi_\perp\xi\overline{w}) + \frac{1}{2}|w|^2)^2 + 4|\psi_\perp|^2|\xi|^2\Re(\psi_\perp\xi\overline{w})\,.$$

Since (4.12) implies that

$$\mathcal{E}^N(\Psi) \geq \omega_\perp + \mathcal{E}_A^N(\xi) - 4g \int_{\mathbb{R}^2 \times]-\frac{NT}{2},\frac{NT}{2}[} |\psi_\perp(x,y)|^3 |\xi(z)|^3 |w(x,y,z)| \, dxdydz \,,$$

in order to get the lower bound, we just need to prove that the last term is a perturbation to $\mathcal{E}_A^N(\xi)$.
We can do the following estimates

$$\begin{aligned} & g \int |\psi_\perp(x,y)|^3 |\xi(z)|^3 |w(x,y,z)| \, dxdydz \\ & \quad \leq c_0 g {\omega_\perp}^{\frac{3}{4}} \left(\int |\psi_\perp(x,y)|^4 \, dxdy\right)^{\frac{3}{4}} \left(\int |\xi(z)|^4 dz\right)^{\frac{3}{4}} \|w\|_4 \\ & \quad \leq c_1 g^{1/4} (\mathcal{E}_A^N(\xi))^{3/4} \|w\|_4 \\ & \quad \leq c_2 g^{1/4} {\delta_\perp}^{-\frac{1}{8}} \left(\tfrac{\delta_\perp + \omega_\perp}{\delta_\perp}\right)^{\frac{1}{4}} \, m_A^N(\epsilon, \widehat{g})^{\frac{1}{2}} (\mathcal{E}_A^N(\xi))^{3/4} \\ & \quad \leq c_3 g^{1/4} {\delta_\perp}^{-\frac{1}{8}} \left(\tfrac{\delta_\perp + \omega_\perp}{\delta_\perp}\right)^{\frac{1}{4}} \, m_A^N(\epsilon, \widehat{g})^{\frac{1}{4}} \left(1 + C\, m_A^N(\epsilon, \widehat{g}) {\delta_\perp}^{-1}\right) \, \mathcal{E}_A^N(\xi) \,. \end{aligned}$$

Here to get the last line, we have used the lower bound

$$\mathcal{E}_A^N(\xi) \geq m_A^N(\epsilon, \widehat{g}) \, ||\xi||_2^4 \,,$$

and (4.15).
This leads to

$$\mathcal{E}^N(\Psi) \geq \omega_\perp + \mathcal{E}_A^N(\xi) \left(1 - C\, g^{1/4} {\delta_\perp}^{-\frac{1}{8}} \left(\frac{\delta_\perp + \omega_\perp}{\delta_\perp}\right)^{\frac{1}{4}} \, m_A^N(\epsilon, \widehat{g})^{\frac{1}{4}} - C\, m_A^N(\epsilon, \widehat{g}) {\delta_\perp}^{-1}\right) ,$$

and then to (4.7).

Remark 4.3.
In the case with rotation Ω, the proof is the same if we replace $\mathcal{E}'_B$ by $\mathcal{E}'_{B,\Omega}$ defined by

$$\mathcal{E}'_{B,\Omega}(\psi) = \int_{\mathbb{R}^2} \left(\frac{1}{2} |\nabla_{x,y} \psi - i\Omega r^\perp \psi|^2 + \frac{1}{2} ({\omega_\perp}^2 - \Omega^2) r^2 |\psi|^2 \right) dxdy \,. \quad (4.21)$$

We also use the diamagnetic inequality

$$\int |\nabla |w|(x,y)|^2 \, dxdy \leq \int |\left(\nabla w - i\Omega r^\perp w\right)(x,y)|^2 \, dxdy \quad (4.22)$$

which provides the Sobolev injections.

Remark 4.4.
Here, we have not proved that the minimizer of $\mathcal{E}$ behaves almost like the ground state in x, y times a function of ξ which minimizes $\mathcal{E}_A$. We are just able (see (4.14)*) to prove that the minimizer is close to its projection (in some L^2 or L^4 norm). When $N = 1$, this can be improved under the stronger condition* (1.49)*. We first observe (note that* (4.13) *is still true with the addition of $\mathcal{E}'_A(\xi)$ on the right hand side) that*

$$\mathcal{E}'_A(\xi) \leq m_A(\epsilon, \widehat{g})\,. \tag{4.23}$$

Using (4.15)*, assuming $\frac{m_A}{\delta_\perp} < 1$, this leads to*

$$\mathcal{E}'_A(\xi) \leq m_A(\epsilon, \widehat{g})(1 - \frac{m_A(\epsilon, \widehat{g})}{\delta_\perp})^{-1}||\xi||^2 \tag{4.24}$$

We will show in Subsection 5.2 (see (5.14)*) how to proceed in order to show that ξ is close to the ground state $\phi_1(z)$ of H_z^{per}.*
This can allow to improve the information given in Theorem 1.2.

5 The $1D$ periodic model : estimates for m_A^N

The aim of this section is to analyze m_A^N. We note that rough estimates were already given for the weak interaction case which were enough for the justification of the model but the corresponding rough estimates needed for the Thomas-Fermi justification will be obtained in this section. We will then look at accurate estimates for m_A^N, which will be established under stronger hypotheses. We will end the section by the discussion of the case $N > 1$, which finally leads to the introduction of the DNLS model for the Weak Interaction case.

5.1 Universal estimates

We consider the one dimensional situation and a T- periodic potential W, which could be for example $W(z) = (\sin \pi z)^2/\epsilon^2$. We consider the problem of minimizing on $L^2(\mathbb{R}/T\mathbb{R})$ the functional

$$\psi \mapsto \mathcal{G}(\psi) = \frac{1}{2}\int_{-\frac{T}{2}}^{\frac{T}{2}} |\psi'(z)|^2\, dz + \int_{-\frac{T}{2}}^{\frac{T}{2}} W(z)|\psi(z)|^2\, dz + \widehat{g}\int_{-\frac{T}{2}}^{\frac{T}{2}} |\psi(z)|^4\, dz\,, \tag{5.1}$$

over $||\psi||_{L^2} = 1$.
We are interested in the control of the minimum of the functional and will simply prove

Lemma 5.1.
If $\widehat{g} \geq 0$, then

$$m(\widehat{g}) := \inf_{||\psi||_{L^2}=1} \mathcal{G}(\psi) = \lambda_1 + \widehat{g} \int_{-\frac{T}{2}}^{+\frac{T}{2}} |\phi_1(z)|^4 \, dz + o(\widehat{g}) \,, \tag{5.2}$$

where (λ_1, ϕ_1) is the spectral pair of $-\frac{1}{2}\frac{d^2}{dz^2} + W(z)$ corresponding to the ground state energy (with $||\phi_1||^2 = 1$).

Proof :
It is clear that

$$\lambda_1 \leq m(\widehat{g}) \leq \lambda_1 + \widehat{g} \int_{-\frac{T}{2}}^{\frac{T}{2}} |\phi_1(z)|^4 dz \,, \tag{5.3}$$

so the question is now to improve the lower bound.
One could of course think of applying bifurcation theory but this gives only a local result and we need in any case a global estimate for showing that the global minimizer of $\mathcal{G}$ is closed to ϕ_1 as $\widehat{g}$ is small.
Let ϕ_{min} be a minimizer of $\mathcal{G}$, then we know that

$$\frac{1}{2} \int_{-\frac{T}{2}}^{\frac{T}{2}} |\phi'_{min}|^2 dz + \int_{-\frac{T}{2}}^{\frac{T}{2}} W(z) |\phi_{min}(z)|^2 \, dz \leq \lambda_1 + \widehat{g} \int_{-\frac{T}{2}}^{\frac{T}{2}} |\phi_1(z)|^4 \, dz \,. \tag{5.4}$$

So ϕ_{min} plays the role of a quasimode (or approximate eigenfunction) for $-\frac{1}{2}\frac{d^2}{dz^2} + W(z)$.
A rather standard theorem in perturbation theory (we can write $\phi_{min} = \alpha \phi_1 + u^\perp$), gives first

$$1 - |\alpha|^2 = ||u^\perp||^2 \leq \widehat{g} \frac{\int_{-\frac{T}{2}}^{\frac{T}{2}} |\phi_1(z)|^4 \, dz}{\lambda_2 - \lambda_1} \,,$$

and then the existence of a complex number c of modulus 1 such that

$$||\phi_{min} - c\phi_1||_{L^2}^2 \leq 2\widehat{g} \frac{\int_{-\frac{T}{2}}^{\frac{T}{2}} |\phi_1(z)|^4 \, dz}{\lambda_2 - \lambda_1} \,. \tag{5.5}$$

Here λ_2 denotes the second eigenvalue of or Hamiltonian.
Of course, the estimate is only interesting if

$$2\widehat{g} \frac{\int_{-\frac{T}{2}}^{\frac{T}{2}} |\phi_1(z)|^4 \, dz}{\lambda_2 - \lambda_1} < 1 \,. \tag{5.6}$$

We can now write

$$
\begin{aligned}
m(\widehat{g}) & \geq \lambda_1 + \widehat{g} \int_{-\frac{T}{2}}^{\frac{T}{2}} |\phi_{min}(z)|^4 \, dz \\
& \geq \lambda_1 + \widehat{g} \int_{-\frac{T}{2}}^{\frac{T}{2}} |\phi_1(z)|^4 \, dz - 4\widehat{g} ||\phi_{min} - c\phi_1||_2 ||\phi_1||_6^3 \, .
\end{aligned}
\tag{5.7}
$$

For the last estimate, we develop $|\phi_{min}|^4$ in the following way

$$
\begin{aligned}
|\phi_{min}|^4 & = |c\phi_1 + \phi_{min} - c\phi_1|^4 \\
& \geq |\phi_1|^4 + 2|\phi_1|^2 |\phi_{min} - c\phi_1|^2 - 4|\phi_1|^3 |\phi_{min} - c\phi_1| \, .
\end{aligned}
\tag{5.8}
$$

From this inequality we get

$$
|\phi_{min}|^4 \geq |\phi_1|^4 - 4|\phi_1|^3 |\phi_{min} - c\phi_1| \, . \tag{5.9}
$$

It just remains to control $||\phi_1||_6$ uniformly with respect to $\widehat{g}$, which can be deduced of the uniform control of the norm of ϕ_1 in L^6. ■

One can actually be more precise on what we have claimed in Lemma 5.1.

Lemma 5.2.
If $\widehat{g} \geq 0$, then

$$
m(\widehat{g}) \geq \lambda_1 + \widehat{g} ||\phi_1||_4^4 - 2^{\frac{5}{2}} \widehat{g}^{\frac{3}{2}} ||\phi_1||_6^3 ||\phi_1||_4^2 (\lambda_2 - \lambda_1)^{-\frac{1}{2}} \, . \tag{5.10}
$$

This estimate is interesting if

$$
\widehat{g} < \frac{1}{32} ||\phi_1||_4^4 ||\phi_1||_6^{-6} (\lambda_2 - \lambda_1) \, . \tag{5.11}
$$

Remark 5.3.
Everything being universal, one can of course replace T by NT in the description.

5.2 Semi-classical results in the Weak Interaction case : $N = 1$

We first recall that using (3.10) we have, under Condition (1.55), the rough control

$$
\frac{1}{C\epsilon} \leq \lambda_{1,z} \leq m_A(\epsilon, \widehat{g}) \leq \lambda_{1,z} + \widehat{g} \int_{-\frac{T}{2}}^{\frac{T}{2}} |\phi_1(z)|^4 \, dz \leq \frac{C}{\epsilon} \, , \tag{5.12}
$$

which leads to (1.57) for $N = 1$ and was sufficient for the justification of the longitudinal model A.

Let us now show that under stronger assumptions one can have a more accurate asymptotics including the main contribution of the non-linear interaction.

Proposition 5.4.
Under Assumption (1.49), m_A *admits the following asymptotics :*

$$m_A(\epsilon, \widehat{g}) = \lambda_1^{har}(\epsilon) + \pi^{-\frac{1}{2}} \mathbf{w}''(0)^{\frac{1}{4}} \widehat{g} \epsilon^{-\frac{1}{2}} + c_0 + \mathcal{O}(\epsilon) + \mathcal{O}(\widehat{g}^{\frac{3}{2}} \epsilon^{-\frac{1}{4}}) . \tag{5.13}$$

Proof :
Indeed, λ_1 and $\lambda_1 - \lambda_2$ are of order $\frac{1}{\epsilon}$, and by (3.10) and (5.5), we get

$$||\phi_{min} - c\phi_1||_{L^2}^2 \leq C \widehat{g} \epsilon^{\frac{1}{2}} . \tag{5.14}$$

Using the harmonic approximation, the term $||\phi_1||_6$ is of order $\epsilon^{-\frac{1}{6}}$ and the remainder appearing in (5.10) is of order $\widehat{g}^{\frac{3}{2}} \epsilon^{-\frac{1}{4}}$. Altogether we get for the energy

$$m_A(\epsilon, \widehat{g}) = \lambda_{1,z} + \widehat{g} \int_{-\frac{T}{2}}^{\frac{T}{2}} |\phi_1(z)|^4 \, dz \ + \mathcal{O}(\widehat{g}^{\frac{3}{2}} \epsilon^{-\frac{1}{4}}) . \tag{5.15}$$

Using (3.10), we obtain (5.13). This asymptotics becomes interesting in the semi-classical regime if (1.49) holds. ■

Remark 5.5.
Exponentially small effects will be discussed in Section 7.

5.3 Semi-classical analysis in a Thomas-Fermi regime : case $N = 1$.

5.3.1 Main results

In this subsection, we first give the rough estimate leading to (1.62) for $N = 1$. Recall that $\widehat{g} = \frac{1}{\pi} g\omega_\perp$, but $\widehat{g}$ and ϵ are taken as independent parameters.

Proposition 5.6.
If for some $c > 0$,

$$\widehat{g} \epsilon^2 \leq c , \tag{5.16}$$

and if
$$\widehat{g}\epsilon^{\frac{1}{2}} >> 1\,, \tag{5.17}$$
then there exist C *and* ϵ_0 *such that*
$$\frac{1}{C}\,\widehat{g}^{\frac{2}{3}}\epsilon^{-\frac{2}{3}} \leq m_A(\epsilon,\widehat{g}) \leq C\widehat{g}^{\frac{2}{3}}\epsilon^{-\frac{2}{3}}\,,\ \forall \epsilon \in]0,\epsilon_0]\,. \tag{5.18}$$

We will also get the following accurate estimate :

Proposition 5.7.
If
$$\widehat{g}\epsilon^2 << 1\,, \tag{5.19}$$
and (5.17) *are satisfied , then*
$$m_A(\epsilon,\widehat{g}) = 2^{-\frac{4}{3}}3^{\frac{5}{3}}5^{-1}\mathbf{w}''(0)^{\frac{2}{3}}\widehat{g}^{\frac{2}{3}}\epsilon^{-\frac{2}{3}}\left(1+\mathcal{O}(\widehat{g}^{-\frac{2}{3}}\epsilon^{-\frac{1}{3}})\right)\,. \tag{5.20}$$

The new asusmption is (5.19), which is stronger than (5.16).

5.3.2 The harmonic functional on $\mathbb{R}$

Let us start with the case of a harmonic potential $W_\epsilon(z) = \gamma\frac{z^2}{2\epsilon^2}$ on $\mathbb{R}$, with $\gamma > 0$, and consider the problem of minimizing
$$q^{Hr,T}(u) = \frac{1}{2}\int_{-\frac{T}{2}}^{\frac{T}{2}} u'(t)^2\,dt + \frac{\gamma}{2\epsilon^2}\int_{-\frac{T}{2}}^{\frac{T}{2}} t^2u(t)^2\,dt + \widehat{g}\int_{-\frac{T}{2}}^{\frac{T}{2}} u(t)^4\,dt \tag{5.21}$$
over the u's in the form domain of $q^{Hr,T}$ such that $||u||^2 = 1$.
We denote by $m_A^{Hr,T}$ the infimum of the functional. Actually there are two approximating " harmonic " functionals of interest corresponding to T finite and to $T = +\infty$. An interesting point is that, for T large enough, the minimizers of these two functionals are the same as we will see below. But let us start with the case $T = +\infty$.

Lemma 5.8.
If (5.17) *holds, then*
$$m_A^{Hr,+\infty}(\epsilon,\widehat{g}) = 2^{-\frac{4}{3}}3^{\frac{5}{3}}5^{-1}\gamma^{\frac{2}{3}}\widehat{g}^{\frac{2}{3}}\epsilon^{-\frac{2}{3}}\left(1+\mathcal{O}(\widehat{g}^{-\frac{2}{3}}\epsilon^{-\frac{1}{3}})\right)\,. \tag{5.22}$$

The proof is very standard (see for example [BBH], [Af] or [CorR-DY] which treat the $(2D)$-case). The analysis is done through a dilation. We look for an L^2-normalized test function ϕ in the form

$$\phi(z) = \rho^{\frac{1}{2}} v(\rho z)\,, \tag{5.23}$$

with ρ and v to be determined.
The $1-D$ energy of ϕ becomes

$$\frac{1}{2}\rho^2 \int_{\mathbb{R}} v'(t)^2 dt + \rho^{-2}\epsilon_\gamma^{-2} \int_{\mathbb{R}} t^2 v(t)^2 dt + \widehat{g}\rho \int_{\mathbb{R}} v(t)^4 dt\,, \tag{5.24}$$

with

$$\epsilon_\gamma = \epsilon / \sqrt{\frac{1}{2}\gamma}\,.$$

This leads to choose $\rho = \rho_\gamma$ such that

$$\rho^{-3} = \widehat{g}\epsilon_\gamma^2\,,$$

hence

$$\rho_\gamma = \epsilon_\gamma^{-\frac{2}{3}} \widehat{g}^{-\frac{1}{3}}\,, \tag{5.25}$$

and the energy of this model becomes

$$\widehat{g}^{\frac{2}{3}} \epsilon^{-\frac{2}{3}} \left(q_{TF}(v) + \frac{1}{2} (\epsilon_\gamma^{\frac{1}{2}} \hat{g})^{-\frac{4}{3}} \int_{\mathbb{R}} v'(t)^2\, dt \right) \tag{5.26}$$

with

$$q_{TF}(v) := \int_{\mathbb{R}} t^2 v(t)^2\, dt + \int_{\mathbb{R}} v(t)^4\, dt\,. \tag{5.27}$$

This is asymptotically of the order of $\widehat{g}^{\frac{2}{3}} \epsilon^{-\frac{2}{3}}$ and Condition (5.17) is just the condition that the kinetic term is negligeable in the computation of the energy.
Let us recall the details of this asymptotics for completeness. We have first to minimize over L^2-normalized v the approximating functional q_{TF}. The minimizer $v_{min}(t)$ of q_{TF} is determined by the equations

$$t^2 v(t) + 2 v(t)^3 = \lambda v(t)\,, \int_{\mathbb{R}} v(t)^2 dt = 1\,. \tag{5.28}$$

We get

$$v_{min}(t) = 2^{-\frac{1}{2}} (\lambda - t^2)_+^{\frac{1}{2}}\,, \tag{5.29}$$

with

$$\lambda = \left(\frac{3}{2}\right)^{\frac{2}{3}}, \tag{5.30}$$

and for $x \in \mathbb{R}$,

$$(x)_+ = \max(x, 0)\,.$$

The corresponding TF-energy is

$$e_{TF} := \int_{\mathbb{R}} (t^2 v_{min}(t)^2 + v_{min}(t)^4)\, dt = \frac{2}{5}\lambda^{\frac{5}{2}}\,. \tag{5.31}$$

Unfortunately, this minimizer is not in $H^1(\mathbb{R})$ and can not be used directly for our initial rescaled functional

$$q^{\sigma}_{TF}(v) = q_{TF}(v) + \sigma \int_{\mathbb{R}} v'(t)^2\, dt\,,$$

with

$$\sigma = \widehat{g}^{-\frac{4}{3}} \epsilon_{\gamma}^{-\frac{2}{3}}\,.$$

Here we recall that (5.17) implies

$$0 \leq \sigma << 1\,.$$

So we need to regularize this minimizer to have an upperbound for the energy of our "harmonic" functional which is good as $\sigma \to 0$.

This can be done in the following way (see for example [Af] and references therein).

We introduce

$$\gamma(s) = \begin{cases} \sqrt{s}\,, & \text{if } s > \sigma^{\frac{1}{3}} \\ s\sigma^{-\frac{1}{6}}\,, & \text{if } s < \sigma^{\frac{1}{3}} \end{cases} \tag{5.32}$$

Let us consider the function

$$\hat{v}_{\sigma}(t) = \gamma(v_{min}(t)^2)\,.$$

We get that $\hat{v}_{\sigma}$ belongs to H^1 and satisfies

$$\int |\hat{v}_{\sigma}(t)|^2\, dt = 1 - r(\sigma)\,,$$

with

$$r(\sigma) = \mathcal{O}(\sigma^{\frac{2}{3}})\,.$$

More precisely the (positive) remainder $r(\sigma)$ is

$$r(\sigma)=\int_{v_{min}(t)^2<\sigma^{\frac{1}{3}}}(-|v_{min}(t)|^2+\sigma^{-\frac{1}{3}}|v_{min}(t)|^4)\,dt\,.$$

Let us now consider as a test function

$$v_\sigma:=\hat{v}_\sigma/\|\hat{v}_\sigma\|\,.$$

Then we have

$$v_\sigma=(1+\frac{1}{2}r(\sigma)+\mathcal{O}(\sigma^{\frac{4}{3}}))\hat{v}_\sigma\,.$$

So we get

$$q^\sigma_{TF}(v_\sigma)=q_{TF}(v_{min})+\mathcal{O}(\sigma\ln\frac{1}{\sigma})\,.$$

So we have the upper-bound in the statement (5.22) (actually with a better remainder term) of the lemma. The lower bound in (5.22) is immediate because the kinetic term is positive.

5.3.3 The harmonic functional on $]-\frac{T}{2},\frac{T}{2}[$

We consider now the case of the interval and have the following Lemma :

Lemma 5.9.
Under Assumption (5.17), *there exists* $C>0$ *such that*

$$m_A^{har,T}(\epsilon,\widehat{g})\geq\frac{1}{C}\,\widehat{g}^{\frac{2}{3}}\epsilon^{-\frac{2}{3}}\,. \tag{5.33}$$

The proof is based on the same method as in the previous subsubsection. It is easy to see that the minimizers coincide if

$$\frac{\rho_\gamma T}{2}>\lambda^{\frac{1}{2}}\,, \tag{5.34}$$

that is

$$T>\widehat{g}^{\frac{1}{3}}\epsilon_\gamma^{\frac{2}{3}}\left(\frac{3}{2}\right)^{\frac{1}{3}}\,. \tag{5.35}$$

If (5.35) is not satisfied, we can still have a lower bound for the infimum of the functional. The renormalized functional reads

$$q^{ren,T}(v):=\rho^2\int_{\frac{\rho T}{2}}^{\frac{\rho T}{2}}v'(t)^2dt+\rho^{-2}\epsilon_\gamma^{-2}\int_{\frac{\rho T}{2}}^{\frac{\rho T}{2}}t^2v(t)^2dt+\widehat{g}\rho\int_{\frac{\rho T}{2}}^{\frac{\rho T}{2}}v(t)^4dt\,, \tag{5.36}$$

which satisfies

$$q^{ren,T}(v) \geq \widehat{g}\rho \left(\int_{\frac{\rho T}{2}}^{\frac{\rho T}{2}} v(t)^4 dt \right) .$$

Using the Hölder inequality, we obtain, if $||v||_2 = 1$,

$$q^{ren,T}(v) \geq (\widehat{g}\rho)(\rho T)^{-1} ,$$

and using our assumption, we obtain

$$q^{ren,T}(v) \geq \frac{1}{2}\lambda^{-\frac{1}{2}}(\widehat{g}\rho) \geq \frac{1}{C}\widehat{g}^{\frac{2}{3}}\epsilon^{-\frac{2}{3}} , \tag{5.37}$$

if $||v||_2 = 1$.

We then immediatly obtain Lemma 5.9.

5.3.4 Relevance of the "harmonic functional" for rough bounds

First we prove Proposition 5.6. We can proceed by direct comparison. Observing that we can find $\alpha > 0$ such that

$$\mathbf{w}(z) \leq \alpha z^2 , \ \forall z \in [-\frac{T}{2}, +\frac{T}{2}] ,$$

and

$$\rho_\alpha T > 2\lambda^{\frac{1}{2}} .$$

Here, we use (5.16) and

$$\rho_\alpha = c_0 \alpha^{\frac{1}{3}} (\epsilon^{-\frac{2}{3}} \widehat{g}^{-\frac{1}{3}}) \geq c_0 \alpha^{\frac{1}{3}} c^{-\frac{1}{3}} .$$

We can then use the asymptotic estimate (5.22) with $\gamma = \alpha$ to get the upper bound in (5.18).

Using now Assumption (1.1), we can also find $\hat{\alpha}$ such that

$$\mathbf{w}(z) \geq \hat{\alpha} z^2 , \ \forall z \in [-\frac{T}{2}, +\frac{T}{2}] ,$$

This leads, using our analysis of q^{TF} in the harmonic case to the lower bound in (5.18).

5.3.5 Relevance of the "harmonic functional' for the asymptotic behavior

In order to have a better localized minimizer, we should assume that $\rho \to +\infty$ and this corresponds to replacing Assumption (5.16) by the stronger Assumption (5.19).

Moreover, we have to verify that under this assumption the "harmonic approximation" is valid for this energy computation. For this, we should analyze the localization of the minimizer. Assuming that such a localized minimizer exists (minimize the functional $v \mapsto \int (z^2 v(z)^2 + v(z)^4)\, dz$), we can also get an upperbound of m_A by using a harmonic approximation and a lower bound of the same order.

For the lower bound, we have just to analyze (forgetting the positive kinetic term) the infimum of the functional

$$\phi \mapsto \int_{-\frac{T}{2}}^{\frac{T}{2}} \left(\frac{\mathbf{w}(z)}{\epsilon^2} \phi^2 + \widehat{g} \phi^4 \right) dz \,.$$

As in the other case, a minimizer (over the L^2-normalized ϕ's), should satisfy, for some $\mu > 0$, the Euler-Lagrange equation

$$\frac{\mathbf{w}(z)}{\epsilon^2} \phi(z) + 2\widehat{g}\phi(z)^3 = \mu \phi(z) \,,$$

where μ will be determined by the L^2 normalization over $]-\frac{T}{2}, \frac{T}{2}[$.
We find

$$\phi(z) = \frac{1}{\sqrt{2\widehat{g}}} \left(\mu - \frac{\mathbf{w}(z)}{\epsilon^2} \right)_+^{\frac{1}{2}} . \tag{5.38}$$

with

$$\frac{1}{2\widehat{g}} \int (\mu - \frac{\mathbf{w}(z)}{\epsilon^2})_+ dz = 1 \,. \tag{5.39}$$

But we know from the upperbound that μ is less than two times the energy which is asymptotically lower than $m_A^{har}(\epsilon \widehat{g})$. In particular, if $\mu \epsilon^2$ is small, it is easy to estimate μ using the harmonic approximation of w at its minimum. It remains to verify the behavior of $\mu \epsilon^2$. We find

$$\mu \epsilon^2 \leq C \widehat{g}^{\frac{2}{3}} \epsilon^{\frac{4}{3}} \,.$$

Not surprisingly, this shows that $\mu \epsilon^2$ is small as $\rho \to +\infty$. So finally, we have obtained Proposition 5.7.

5.4 The case $N > 1$

We would like to extend our rough or accurate estimates for m_A to the analogous estimates for $N > 1$, keeping the same kind of assumptions.

5.4.1 Universal control

We now consider the functional over $]-\frac{NT}{2}, \frac{NT}{2}[$. Using the minimizer obtained for $N = 1$ and extending it by periodicity, we get after renormalization, the general upper-bound

$$m_A^N(\epsilon, \widehat{g}) \leq m_A(\epsilon, \frac{\widehat{g}}{N})\,. \tag{5.40}$$

From this comparison, we obtain immediately the rough upper bounds in the WI case and in the TF case.

5.4.2 Rough lower bounds

In the WI case, we always have, observing that $\lambda_{1,z}$ is the ground state energy for any $N \in \mathbb{N}^*$,

$$\lambda_1^z \leq m_A^N(\epsilon, \widehat{g})\,. \tag{5.41}$$

Hence we obtain in full generality

Proposition 5.10.
Under Condition (1.54), then, for any $N \geq 1$, we have

$$m_A^N(\epsilon, \widehat{g}) \approx \frac{1}{\epsilon} \tag{5.42}$$

In the TF case, it remains to prove the lower bound which will be a consequence of the following inequality :

$$m_A^N(\epsilon, \widehat{g}) \geq \frac{1}{CN^2} \widehat{g}^{\frac{2}{3}} \epsilon^{\frac{4}{3}}\,. \tag{5.43}$$

We indeed observe that if u_N is a normalized minimizer, then there exists one interval $I_j :=]j\frac{T}{2}, (j+2)\frac{T}{2}[$ ($j \in \{-N, \ldots, N-2\}$), such that

$$\int_{I_j} |u_N|^2 \, dz \ \geq \frac{1}{N}$$

We can then write, forgetting the kinetic term and translating I_j to $]-\frac{T}{2},+\frac{T}{2}[$,

$$\begin{aligned} m_A^N(\epsilon,\widehat{g}) &\geq \epsilon^{-2}\int_{I_j}\mathbf{w}(z)\,|u_N|^2\,dz+\widehat{g}\int_{I_j}|u_N|^4\,dz \\ &\geq \inf(||u_N||^2,||u_N||^4)\inf_{||u||=1}\int_{-\frac{T}{2}}^{+\frac{T}{2}}(W_\epsilon|u|^2+\widehat{g}|u|^4)\,dz\,. \end{aligned}$$

Then we can combine the lower bound obtained for $N=1$ and the inequality $\mathbf{w}(z)\geq\hat{\alpha}z^2$ to get (5.43). So we get finally that m_A^N has the right order in the TF case.

Proposition 5.11.
Under Assumptions (5.16) *and* (5.17), *we have, for any* $N\geq 1$,

$$m_A^N(\epsilon,\widehat{g})\approx\widehat{g}^{\frac{2}{3}}\epsilon^{\frac{4}{3}}\,. \tag{5.44}$$

This extends to general N our former Proposition 5.6.

5.4.3 Asymptotics

We would like to give conditions under which the universal upperbound (5.40) becomes actually asymptotically or exactly a lower bound.

Proposition 5.12.
Under either Assumption (1.49) *or Assumptions* (5.17) *and* (5.19),

$$m_A^N(\epsilon,\widehat{g})\sim m_A(\epsilon,\frac{\widehat{g}}{N})\,. \tag{5.45}$$

Proof :
The upperbound was already obtained in (5.40). The proof of the lower bound is different in the two considered cases.

WI case. We will see later (in (7.6)) by a rough analysis of the tunneling effect and the property that the infimum of the function

$$\mathcal{C}^N\ni(c_0,c_2,\ldots,c_{N-1})\mapsto\sum_{j=0}^{N-1}|c_j|^4$$

over $\sum_j |c_j|^2 = 1$ is attained when all the $|c_j|$'s are equal :

$$|c_j| = \frac{1}{\sqrt{N}}\,, \quad \text{for } j = 0, \ldots, N-1\,, \tag{5.46}$$

that, under Assumption (1.49), there exist $C > 0$, $\epsilon_0 > 0$ and $\alpha > 0$ such that

$$m_A^N(g,\epsilon) \geq m_A(\frac{\widehat{g}}{N},\epsilon) - C(\widehat{g}+1)\exp -\frac{\alpha}{\epsilon}\,, \ \forall \epsilon \in (0,\epsilon_0]\,. \tag{5.47}$$

TF case. In this case we can for the lower bound forget the kinetic term and come back to the analysis of Subsubsection 5.3.5, with T replaced by NT. Under Assumption (5.19), we have seen in (5.38) that the minimizer u_N is localized in the neighborhood of each minimum and T-periodic.
We can then write

$$\begin{aligned}
\int_{-\frac{NT}{2}}^{\frac{NT}{2}} \left(\tfrac{\mathbf{w}}{\epsilon^2}|u_N|^2 + \widehat{g}|u_N|^4\right)\, dz \ &= N\int_{-\frac{T}{2}}^{\frac{T}{2}} \left(\tfrac{\mathbf{w}}{\epsilon^2}|u_N|^2 + \widehat{g}|u_N|^4\right)\, dz \\
&= \int_{-\frac{T}{2}}^{\frac{T}{2}} \left(\tfrac{\mathbf{w}}{\epsilon^2}|\sqrt{N}u_N|^2 + \tfrac{\widehat{g}}{N}|\sqrt{N}u_N|^4\right)\, dz \\
&\geq \inf_{||v||=1}\int_{-\frac{T}{2}}^{\frac{T}{2}} \left(\tfrac{\mathbf{w}}{\epsilon^2}|v|^2 + \tfrac{\widehat{g}}{N}|v|^4\right)\, dz\,.
\end{aligned}$$

But under Assumptions (5.17) and (5.19), the last term in the inequality has same asymptotics as $m_A(\epsilon, \frac{\widehat{g}}{N})$ and we are done.

■

Remark 5.13.
This proposition leaves open the question of the equality in (5.45).

6 Study of Case (B) : Justification of the transverse reduced model

6.1 Main result

We have defined $\mathcal{E}_{B,\Omega}^N$ by (1.40)-(1.41) and $m_{B,\Omega}^N$, the infimum of the energy by (1.52). In case B, the proof of the reduction does not depend on whether $N = 1$ or $N > 1$. The only difference is when looking at the rough or accurate estimates of the reduced model. Note that only rough estimates are used in the part concerning the justification of the model.

The reduction is very similar to case A, and we will prove

Theorem 6.1.
If

$$(RBa) \quad \epsilon\, m^N_{B,\Omega} << 1\,, \tag{6.1}$$

and

$$(RBb) \quad g\, m^N_{B,\Omega}\, \epsilon^{\frac{1}{2}} << 1\,, \tag{6.2}$$

then, as ϵ *tends to* 0,

$$\inf_{||\Psi||=1} Q^{per,N}_{\Omega}(\Psi) = \lambda_{1,z} + m^N_{B,\Omega}(1+o(1))\,. \tag{6.3}$$

Then Theorems 1.5 and 1.6 follow from this result and appropriate estimates on $m^N_{B,\Omega}$, as we will prove in section 6.2, while the proof of Theorem 6.1 is made in Section 6.3.

6.2 Proof of Theorems 1.5 and 1.6

The issue is to determine the magnitude of the infimum of the energy of the transverse problem $m^N_{B,\Omega}$.

6.2.1 Reduction to the case $N=1$

As in Case A it is immediate to see that

$$m^N_{B,\Omega} \leq m_{B,\Omega}(\frac{\widetilde{g}}{N}, \omega_\perp)\,. \tag{6.4}$$

If indeed $\psi_{min,N}$ was the T-periodic minimizer for (1.38) with $\widetilde{g}_N = \frac{\widetilde{g}}{N}$, we get (6.4) by using (1.26), (2.27) and taking $\psi_{j,\perp} = \frac{1}{\sqrt{N}}\psi_{min,N}$.

So it remains for the needed upper-bound to analyze the case $N=1$. This depends on the magnitude of $\tilde{g}$ and leads us to consider two cases.

6.2.2 The Weak Interaction regime : case $N=1$

Proposition 6.2.
If (1.66) holds, then

$$m_{B,\Omega}(\widetilde{g}, \omega_\perp) \leq C\omega_\perp\,. \tag{6.5}$$

Indeed, (1.66) implies that $\tilde{g}$ is bounded and the test function $\psi_\perp$ (which is independent of Ω) implies the proposition.

Therefore, if (1.66) and (1.67) are satisfied, then Theorem 6.1 holds and implies Theorem 1.5.

6.2.3 The Thomas Fermi regime : case $N = 1$

We start with the case when $\Omega = 0$. When $\tilde{g}$ is not bounded, we can meet a Thomas-Fermi situation.

Proposition 6.3.
If $\widetilde{g} \to +\infty$, the function $m_B(\widetilde{g}, \omega_\perp)$ satisfies

$$m_B(\widetilde{g}, \omega_\perp) \sim c_{TF}\omega_\perp\sqrt{\widetilde{g}}\,, \tag{6.6}$$

with

$$c_{TF} = \frac{\pi}{24}\lambda^3 = 3^{-1}2^{\frac{3}{2}}\pi^{-\frac{1}{2}}\,. \tag{6.7}$$

Therefore, if (1.70), (1.71), (1.72) are satisfied, then Theorem 6.1 implies Theorem 1.6.

Proof.
A rescaling in $\sqrt{\sqrt{\widetilde{g}}/\omega_\perp}$ yields a new energy

$$u \mapsto \frac{\omega_\perp}{2}\int_{\mathbb{R}^2}\left(\frac{1}{\sqrt{\widetilde{g}}}|\nabla u|^2 + \sqrt{\widetilde{g}}r^2|u|^2 + 2\sqrt{\widetilde{g}}|u|^4\right)dxdy\,,$$

which is of the type Thomas Fermi (that is kinetic energy can be neglected) if

$$\frac{1}{\sqrt{\widetilde{g}}} << \sqrt{\widetilde{g}}\,. \tag{6.8}$$

This leads then simply to the TF reduced functional

$$u \mapsto (\omega_\perp\sqrt{\widetilde{g}})\int_{\mathbb{R}^2}\left(\frac{1}{2}r^2|u|^2 + |u|^4\right)\,dxdy\,,$$

whose infimum over the unit ball in $L^2(\mathbb{R}^2)$ is of order $c_{TF}(\omega_\perp\sqrt{\widetilde{g}})$, with $c_{TF} > 0$ defined by :

$$c_{TF} = \inf_{||u||_2=1}\int_{\mathbb{R}^2}\left(\frac{1}{2}r^2|u(x,y)|^2 + |u(x,y)|^4\right)\,dxdy\,. \tag{6.9}$$

The minimizer exists and is explicitly known as

$$u_{min}(x,y) = \frac{1}{2}(\lambda - r^2)_+^{\frac{1}{2}} \text{ with } \lambda = 2^{\frac{3}{2}}\pi^{-\frac{1}{2}}\,.$$

This leads to (6.7).

In addition, by a computation similar to the one in Subsection 5.3, we obtain more precisely

Lemma 6.4.
There exists c such that, as $\widetilde{g}$ tends to $+\infty$,

$$\frac{m_B}{\omega_\perp} = c_{TF}\,\sqrt{\widetilde{g}} + \frac{c}{\sqrt{\widetilde{g}}}\ln\widetilde{g} + \mathcal{O}(\frac{1}{\sqrt{\widetilde{g}}})\,, \tag{6.10}$$

with c_{TF} defined in (6.9)*.*

Remark 6.5.
Note that we have the universal lower bound

$$m_B(\widetilde{g},\omega_\perp) \geq c_{TF}\,\omega_\perp\sqrt{\widetilde{g}}\,. \tag{6.11}$$

This lower bound becomes better than the universal lower bound by $\omega_\perp$ as soon as

$$c_{TF}\,\sqrt{\widetilde{g}} > 1\,. \tag{6.12}$$

Remark 6.6.
In the semi-classical regime, conditions (BTFa) and (BTFc) in Theorem 1.6 (take their product) imply that this two-dimensional energy is much smaller than $1/\epsilon$, that is

$$\omega_\perp g^{\frac{1}{2}}\epsilon^{-1/4} << \epsilon^{-1}\,. \tag{6.13}$$

We now look at the case when $\Omega > 0$. The previous proof, using that the minimizer of the TF reduced functional in (6.9) is radial, yields

Proposition 6.7.
There exists C such that, as $\widetilde{g} \to +\infty$,

$$m_{B,\Omega}(\widetilde{g},\omega_\perp) \leq m_B(\widetilde{g},\omega_\perp) + C\ln\widetilde{g}\;\widetilde{g}^{-\frac{1}{2}}\,. \tag{6.14}$$

This will be improved in (6.48) by a direct study of the minimizer of $\mathcal{E}_{B,\Omega}$.

Remark 6.8.
For a lower bound, we can use the TF reduced functional

$$I_\Omega(u) = \omega_\perp \sqrt{\widetilde{g}} \int_{\mathbb{R}^2} \left(\frac{1}{2}(1 - \Omega^2/{\omega_\perp}^2) r^2 |u|^2 + |u|^4 \right) dxdy$$

whose minimum is explicit :

$$\inf_{||u||=1} I_\Omega(u) = \omega_\perp \sqrt{\widetilde{g}} e_{TF} \sqrt{\frac{1}{2}(1 - \Omega^2/{\omega_\perp}^2)}\,.$$

Thus we get that, if there exists $\beta \in [0,1[$ such that

$$0 \leq \Omega/\omega_\perp \leq \beta\,, \tag{6.15}$$

then, as $\widetilde{g} \to +\infty$,

$$m_{B,\Omega}(\widetilde{g}, \omega_\perp) \approx \omega_\perp \sqrt{\widetilde{g}}\,. \tag{6.16}$$

The uniformity of the approximation depends on β.

In fact, if one wants a more precise expansion of the energy, one can use the ground state ρ of I_Ω to split the energy $\mathcal{E}_{B,\Omega}(u)$. Indeed the Euler Lagrange equation for ρ multiplied by $(1 - |u|^2)$ for any function u yields the identity (see [Af])

$$\mathcal{E}_{B,\Omega}(u) = I_\Omega(\rho) + \int \rho^2 |\nabla v - i\Omega \times rv|^2 + \tilde{g}\rho^4 (1 - |v|^2)^2$$

where $v = u/\rho$. Thus, I_Ω always provides a lower bound with an inverted parabola profile as soon as we are in a TF situation. The second part of the energy has the vortex contribution which is of lower order when $\Omega/\omega_\perp << 1$. More precisely, the first vortex is observed for a velocity Ω of order $\omega_\perp \ln \tilde{g}/\sqrt{\tilde{g}}$. When Ω increases and becomes at most like $\beta\omega_\perp$ with $\beta < 1$, the two parts of the energy $I(\rho)$ and the rest become of similar magnitude. In the limit, $\Omega \to \omega_\perp$, there are a lot of vortices and the description can be made with the lowest Landau levels sets of states. The leading order term of the energy is the first eigenvalue of $-(\nabla - i\Omega \times r)^2$ which is equal to Ω.

6.3 Proof of Theorem 6.1

We recall that we have the universal upperbound (1.64). The lower bound follows from the following proposition and the fact that there exists $c > 0$ such that

$$\delta_z^N \sim c/\epsilon\,,$$

as ϵ tends to 0.

Proposition 6.9.
There exists a universal constant $C > 0$ such that

$$\inf_{||\Psi||=1} Q_\Omega^{per,N}(\Psi) = \lambda_{1,z} + m_{B,\Omega}^N \,(1 - C r_B^N)\,. \tag{6.17}$$

with

$$0 \leq r_B^N \leq m_{B,\Omega}^N (\delta_z^N)^{-1} + g^{\frac{1}{4}} (\delta_z^N)^{-\frac{1}{8}} (m_{B,\Omega}^N)^{\frac{1}{4}} (1 + \frac{\lambda_{1,z}}{\delta_z^N})^{\frac{1}{8}}\,. \tag{6.18}$$

Before giving the detailed proof, let us shortly sketch the case $N = 1$. The proof is indeed essentially the same as for Case (A). One has just to exchange the role of (A) and (B). m_A should be replaced by m_B, $\omega_\perp$ by $\lambda_{1,z}$ and δ_z by $\delta_\perp$. Note that in the two models (A) and (B) the ratio between the ground state energy and the splitting is of order 1. We have indeed

$$\delta_\perp = \omega_\perp \text{ and, in the semi-classical regime, } \frac{\lambda_{1,z}}{\delta_z} \approx 1\,.$$

Proof :
We start from a minimizer Ψ and first write

$$\Psi = \Pi_N \Psi + w \tag{6.19}$$

where Π_N is the projection relative to the first N eigenfunctions of H_z introduced in (1.33). We have

$$\Pi_N w = 0\,, \tag{6.20}$$

and

$$||w||^2 + ||\Pi_N \Psi||^2 = 1\,. \tag{6.21}$$

We have the lower bound

$$\int_{\mathbb{R}^2_{x,y}} \mathcal{E}'_A(w)\, dxdy \geq \lambda_{N+1,z} \int_{\mathbb{R}^2 \times]-\frac{NT}{2}, +\frac{NT}{2}[} |w(x,y,z)|^2 dxdydz\,, \tag{6.22}$$

with

$$\mathcal{E}'_A(\phi) := \int_{-\frac{NT}{2}}^{\frac{NT}{2}} \left(\frac{1}{2} \phi'(z)^2 + \frac{1}{\epsilon^2} \mathbf{w}(z) \phi(z)^2 \right)\, dz\,. \tag{6.23}$$

We now rewrite the energy in the form

$$Q_\Omega^{per,N}(\Psi) = \int_{-\frac{NT}{2}}^{\frac{NT}{2}} \mathcal{E}'_{B,\Omega}(\Psi)\, dz + \int_{\mathbb{R}^2_{x,y}} \mathcal{E}'_A(\Pi_N \Psi)\, dxdy + \int_{\mathbb{R}^2_{x,y}} \mathcal{E}'_A(w)\, dxdy + I_N(\Psi)\,, \tag{6.24}$$

with

$$I_N(\Psi) = g \int |\Psi|^4 dxdydz\,, \tag{6.25}$$

and

$$\mathcal{E}'_{B,\Omega}(\psi) = \int_{\mathbb{R}^2_{x,y}} \left(\frac{1}{2}|\nabla_{x,y}\psi - i\Omega r_\perp \psi|^2 + \frac{1}{2}({\omega_\perp}^2 - \Omega^2) r^2 |\psi|^2\right) dxdy\,, \tag{6.26}$$

with $r_\perp = (-y, x)$.

We note that $I_N \geq 0$ and that

$$\mathcal{E}'_{B,\Omega}(\psi) \geq \omega_\perp ||\psi||^2\,. \tag{6.27}$$

We first get the control of $||w||^2$. Having in mind (1.64), we obtain

$$\begin{aligned} \lambda_{1,z} + m^N_{B,\Omega} \quad & \geq Q^{per,N}_\Omega(\Psi) \\ & \geq \omega_\perp + \lambda_{N+1,z}||w||^2 + \lambda_{1,z}||\Pi_N \Psi||^2 \end{aligned} \tag{6.28}$$

and this implies

$$||w||^2 \leq \frac{m^N_{B,\Omega}}{\delta^N_z}\,. \tag{6.29}$$

The right hand side in (6.29) is small according to (6.1). Note also that we have immediately from (6.21),

$$||\Pi_N \Psi||^2 \geq 1 - \frac{m^N_{B,\Omega}}{\delta^N_z}\,. \tag{6.30}$$

We now have to control the derivatives of w. For the transverse control, we start from

$$\lambda_{1,z} + m^N_{B,\Omega} \geq \lambda_{1,z} + \frac{1}{2}\int_{\mathbb{R}^2_{x,y}\times]-\frac{NT}{2},\frac{N}{2}} |\nabla_{x,y} w - i\Omega r_\perp w|^2 dxdy\,, \tag{6.31}$$

which leads to

$$|||\nabla_{x,y} w - i\Omega r_\perp w|\,||^2 \leq 2 m^N_{B,\Omega}\,. \tag{6.32}$$

For the longitudinal control, we write, for any $\alpha \in [0, 1]$

$$\lambda_{1,z} + m^N_{B,\Omega} \geq \lambda_{1,z}||\Pi_N \Psi||^2 + \frac{\alpha}{2}||\partial_z w||^2 + \lambda_{N+1,z}(1-\alpha)||w||^2\,. \tag{6.33}$$

We determine α by writing

$$\lambda_{N+1,z}(1-\alpha) = \lambda_{1,z}\,,$$

hence

$$\alpha = 1 - \frac{\lambda_{1,z}}{\lambda_{N+1,z}}\,. \tag{6.34}$$

So we have

$$||\partial_z w||^2 \leq \frac{2}{\alpha} m^N_{B,\Omega} \leq 2\frac{\lambda_{N+1,z}}{\delta_{N,z}} m^N_{B,\Omega}\,. \tag{6.35}$$

In the semi-classical regime where we are, this leads to the existence of a constant C such that

$$||\partial_z w||^2 \leq C m^N_{B,\Omega}\,. \tag{6.36}$$

Using in addition the diamagnetic inequality, we obtain

$$||\nabla |w|||_2^2 \leq C m^N_{B,\Omega}\,. \tag{6.37}$$

As in the other case, we obtain from Sobolev's Inequality the control of w in L^6 norm

$$||w||_6 \leq C(m^N_{B,\Omega})^{\frac{1}{2}}(1 + \frac{1}{\delta^N_z})^{\frac{1}{3}} \leq \widetilde{C}(m^N_{B,\Omega})^{\frac{1}{2}}\,, \tag{6.38}$$

where we have used that $\delta^N_z >> 1$ in the semi-classical regime.
Using Hölder's inequality, we obtain

$$||w||_4 \leq C(m^N_{B,\Omega})^{\frac{1}{2}}(\delta^N_z)^{-\frac{1}{8}}\,. \tag{6.39}$$

We now have all the estimates needed to mimic the proof of case A.

We start from

$$\mathcal{E}(\Psi) \geq \lambda_{1,z} + \mathcal{E}_B(\Pi_N\Psi) - 4g\int |\Pi_N\Psi|^3|w|\; dxdydz\,. \tag{6.40}$$

We have now to control the third term in (6.40) by the second term. This is done like in case A in the following way :

$$\begin{aligned} 4g\int |\Pi_N\Psi|^3|w|\; dxdydz \; &\leq 4g||\Pi_N\Psi||_4^3\; ||w||_4 \\ &\leq C_1 g^{\frac{1}{4}}(\delta^N_z)^{-\frac{1}{8}}\,(\mathcal{E}_B(\Pi_N\Psi))^{\frac{3}{4}}\;(m^N_{B,\Omega})^{\frac{1}{2}}\,. \end{aligned} \tag{6.41}$$

We now use

$$\mathcal{E}_B(\Pi_N\Psi) \geq m^N_{B,\Omega}||\Pi_N\Psi||_2^4\,, \tag{6.42}$$

which together with (6.29) leads to

$$m^N_{B,\Omega} \leq C(1 + \frac{m^N_{B,\Omega}}{\delta^N_z})\mathcal{E}_B(\Pi_N\Psi)\,. \tag{6.43}$$

This leads to

$$4g \int |\Pi_N \Psi|^3 |w| \, dxdydz \leq C_2 g^{\frac{1}{4}} (m_{B,\Omega}^N)^{\frac{1}{4}} (\delta_z^N)^{-\frac{1}{8}} (1+\frac{m_{B,\Omega}^N}{\delta_z^N}) \mathcal{E}_B(\Pi_N \Psi)\,. \quad (6.44)$$

Using this control, (6.29), (6.40) and (6.42), we have obtained the detailed proof of (6.17) in the general case.

■

6.4 On the minimizers of $\mathcal{E}_B$.

The next proposition is rather standard and refers to the case $N = 1$ but has its own interest. As a corollary, this will yield an upperbound for $m_{B,\Omega}$.

Proposition 6.10.
The minimizer of $\mathcal{E}_B$ over the normalized ψ's is unique (up to a multiplicative constant of modulus 1) and radial.

Proof :
We first observe that if ψ is a minimizer then $|\psi|$ is also a minimizer. Consequently, we start considering a non negative minimizer.
Now $|\psi|$ is solution of the corresponding Euler equation and by the Maximum Principle, $|\psi|$ cannot have a local minimum. Hence ψ cannot vanish and we can write

$$\psi = |\psi| \, e^{i\alpha} \,.$$

Comparing $\mathcal{E}_B(\psi)$ and $\mathcal{E}_B(|\psi|)$ we get

$$|\nabla \psi| = |\nabla |\psi| \,| \; a.e.$$

and this implies that α is constant.
So we can now assume that ψ is a real positive minimizer. The Euler-Lagrange equation reads

$$-\Delta \psi + {\omega_\perp}^2 r^2 \psi + g|\psi|^2 \psi = \lambda \psi \quad (6.45)$$

for some real Lagrange multiplier λ.
Let ϕ another positive solution (with $||\phi||_{L^2} = 1$) of the Euler-Lagrange equation for a possibly different $\mu \in \mathbb{R}$:

$$-\Delta \phi + {\omega_\perp}^2 r^2 \phi + g|\phi|^2 \phi = \mu \phi \,. \quad (6.46)$$

Possibly exchanging the roles of ψ and ϕ, we can w.l.o.g assume that

$$\lambda \geq \mu\,.$$

Let us consider, for some $\alpha > 0$ to be determined, the rescaling

$$\phi(x,y) = \sqrt{\alpha}\, u(\sqrt{\alpha}x, \sqrt{\alpha}y)\,,$$

we get for u the equation

$$-\Delta u + \frac{{\omega_\perp}^2}{\alpha^2} r^2 u + g|u|^2 u = \frac{\mu}{\alpha} u\,.$$

We now choose $\alpha = \frac{\mu}{\lambda}$ which leads to

$$-\Delta u + {\omega_\perp}^2 \left(\frac{\lambda^2}{\mu^2}\right) r^2 u + g|u|^2 u = \lambda u\,. \tag{6.47}$$

We can now compare u and ψ. Let us introduce $v = \frac{u}{\psi}$ which is a solution of

$$-\mathrm{div}\,\left(\psi^2 \nabla v\right) + g v \psi^4 (|v|^2 - 1) = {\omega_\perp}^2 r^2 v \psi^2 (1 - \frac{\lambda^2}{\mu^2})\,.$$

Multiplying by $(v-1)_+$ and integrating[7] we obtain

$$\int_{\mathbb{R}^2} \psi^2 |\nabla (v-1)_+|^2 + g v \psi^4 (v-1)_+^2 (v+1)\; dxdy = \int_{\mathbb{R}^2} {\omega_\perp}^2 r^2 v \psi^2 (1 - \frac{\lambda^2}{\mu^2})\; dxdy\,.$$

With our assumption on (λ, μ), this implies the vanishing of $(v-1)_+$ almost everywhere hence $v \leq 1$.
This can be reinterpreted as $u \leq \psi$ and the L^2 normalization implies $u = \psi$. The lemma is proved.

Finally, one can construct a radial positive solution (by minimizing $\mathcal{E}_B$ over the radial functions). This gives a solution ϕ of the Euler equation which is also strictly positive. ∎

Observing that, if ψ is radial, we have that $\mathcal{E}_{B,\Omega}(\psi) = \mathcal{E}_B(\psi)$, this proposition has the following interesting corollary.

Corollary 6.11.
We always have

$$\inf \mathcal{E}_{B,\Omega} := m_{B,\Omega} \leq m_B\,. \tag{6.48}$$

[7] In full rigor, we should consider a sequence $\chi_n (v-1)_+$ where $(\chi_n)_n$ is a suitable sequence of cut-off functions and take the limit (See [BrOs]).

6.5 Lower bounds in the TF case ($N \geq 1$)

We start from a minimizer $(\psi_{\ell,\perp})_\ell$. Due to the normalization, there exists at least one j such that

$$||\psi_{j,\perp}|| \geq \frac{1}{\sqrt{N}}$$

Then we write (neglecting the kinetic part)

$$m^N_{B,\Omega} \geq \frac{1}{2}(\omega^2-\Omega^2)\int r^2|\psi_{j,\perp}|^2 + g\int_{-\frac{NT}{2}}^{\frac{NT}{2}}\int_{\mathbb{R}^2_{x,y}}\left(\sum_{j=0}^{N-1}\psi_j^N(z)\psi_{j,\perp}(x,y)\right)^4 dzdxdy\,.$$

When expanding $\left(\sum_{j=0}^{N-1}\psi_j^N(z)\psi_{j,\perp}(x,y)\right)^4$, the mixed terms are exponentially small (see Subsection 7.1) in comparison to $\sum_j ||\psi_{j,\perp}||^4_{L^4}$, hence we get, for some $\alpha > 0$,

$$m^N_{B,\Omega} \geq \frac{1}{2}(\omega^2-\Omega^2)\int r^2|\psi_{j,\perp}|^2 + g\int_{-\frac{NT}{2}}^{\frac{NT}{2}}\psi_0^N(z)^4dz(\int(\psi_{j,\perp})^4dxdy)\,(1-\exp-\frac{\alpha}{\epsilon})\,.$$

We now use (7.4), to obtain

$$\begin{array}{rl} m^N_{B,\Omega} & \geq \frac{1}{2}(\omega^2-\Omega^2)\int r^2|\psi_{j,\perp}|^2 + g\int_{-\frac{T}{2}}^{\frac{T}{2}}\phi_1(z)^4dz(\int\psi_{j,\perp}^4dxdy)(1-\exp-\frac{\alpha}{\epsilon}) \\ & = \frac{1}{2}(\omega^2-\Omega^2)\int r^2|\psi_{j,\perp}|^2 + \widetilde{g}(\int\psi_{j,\perp}^4dxdy)(1-\exp-\frac{\alpha}{\epsilon}) \\ & \geq \left(\frac{1}{2}(\omega^2-\Omega^2)\int r^2|\psi_{j,\perp}|^2 + \widetilde{g}(\int\psi_{j,\perp}^4dxdy)\right)(1-\exp-\frac{\alpha}{\epsilon}) \\ & \geq \frac{1}{N^2}(1-\exp-\frac{\alpha}{\epsilon})\inf_{\psi,||\psi||=1}\left(\frac{1}{2}(\omega^2-\Omega^2)\int r^2|\psi|^2 + \widetilde{g}(\int\psi^4dxdy)\right)\,. \end{array}$$

One can then use the asymptotics obtained in the proof of (6.16) to get, under Assumption (6.15), the existence of $C_{N,\beta} > 0$ such that, as ϵ tends to 0 and $\widetilde{g}$ to ∞,

$$m^N_{B,\Omega} \geq \frac{1}{C_{N,\beta}}\omega_\perp\sqrt{\widetilde{g}}\,. \tag{6.49}$$

7 Tunneling effects for the non-linear models

This is only in this section that we will exhibit the role of these localized (NT)-periodic Wannier functions.

7.1 Towards the DNLS model.

7.1.1 Preliminaries

We have already proved for any $N \geq 1$ the rough estimates on m_A^N allowing to justify the longitudinal model. We have established or announced better asymptotics at the price of stronger assumptions.
Our aim in this section is to discuss possible asymptotics for m_A^N in the case when $N > 1$, which will involve the tunneling effect. Although we have no final result on this part, we would like to prove how we reach a familiar model considered by the physicists : the DNLS model.
In particular we will describe in Proposition 7.7 under which assumptions one can get a simplified model.

We consider on $]-\frac{NT}{2}, \frac{NT}{2}[$ the (NT)-periodic problem for the operator $-\frac{d^2}{dz^2} + W_\epsilon(z)$ with $W_\epsilon(z) = \frac{\mathbf{w}(z)}{\epsilon^2}$, w satisfying Assumption (1.1). Here we always work in the semi-classical regime.

The starting point in this subsection is that we replace the issue of minimizing $\mathcal{E}_A^{N,\epsilon,\widehat{g}}$ on the (NT)-periodic L^2-normalized functions by restricting the approximation to the eigenspace $\operatorname{Im}\pi_N$ associated with the first N eigenvalues of the linear problem.

7.1.2 Projecting on the eigenspace $\operatorname{Im}\pi_N$

Our aim is to analyze the reduced functional

$$\mathbb{C}^N \ni \mathbf{c} = (c)_{j=0,\ldots,N-1} \mapsto \mathcal{E}_A^{N,\epsilon,\widehat{g},red}(\mathbf{c}) = \mathcal{E}_A^{N,\epsilon,\widehat{g}}(\sum_{j=0}^{N-1} c_j \psi_j^N)\,, \tag{7.1}$$

where $\mathcal{E}_A^{N,\epsilon,\widehat{g}}$ is in fact $\mathcal{E}_A^N$ given in (1.35) with the explicit notation of the dependence of the parameters and the ψ_j^N are the (NT)-periodic Wannier functions. When $N = 1$, the error which is done has been estimated in (5.15) under the assumption that $\widehat{g}\epsilon^{\frac{1}{2}}$ is small, i.e. (1.49). Replacing in the argument the projection on the first eigenspace by π_N, the same result holds true for $N > 1$.

We now concentrate our discussion to the model obtained after this first approximation. More specifically we are interested in the asymptotics of the infimum of this functional.

Here natural approximations of this reduced functional appear. Each of these approximations gives a corresponding approximation of the infimum of the reduced functional, which is defined by :

$$m_A^{N,(0)}(\epsilon,\widehat{g}) := \inf_{\{\mathbf{c}\,|\,\sum_{j=0}^{N-1}|c_j|^2=1\}} \mathcal{E}_A^{N,\epsilon,\widehat{g},red}(\mathbf{c})\,. \tag{7.2}$$

Let $\lambda_{1,z}^N = \lambda_{1,z}$ be the bottom of the (NT)-periodic spectrum of H_z on $[-\frac{NT}{2},\frac{NT}{2}]$ (with N minima). So strictly speaking, we can start the analysis of this first approximate model only under Condition (1.49).

Proposition 7.1.
Under condition (1.49)

$$m_A^N(\epsilon,\widehat{g}) = m_A^{N,(0)}(\epsilon,\widehat{g}) + \mathcal{O}(\widehat{g}^{\frac{3}{2}}\epsilon^{-\frac{1}{4}})\,. \tag{7.3}$$

One can nevertheless imagine that the information obtained in the next subsubsection is valid in a more general context (maybe by choosing other localized Wannier functions). We now analyze various approximations of $m_A^{N,(0)}(\epsilon,\widehat{g})$.

7.1.3 Neglecting the tunneling

Neglecting the tunneling effect, we are lead to the minimum of the functional $\mathcal{E}_A^{N,\epsilon,\widehat{g},(1)}$

$$\mathbb{C}^N \ni \mathbf{c} \mapsto \mathcal{E}_A^{N,\epsilon,\widehat{g},(1)}(\mathbf{c}) := \lambda_{1,z}\left(\sum_{j=0}^{N-1}|c_j|^2\right) + \widehat{g}\,(\sum_{j=0}^{N-1}|c_j|^4)\,(\int_{-\frac{NT}{2}}^{\frac{NT}{2}}|\psi_0^N(z)|^4\,dz)\,,$$

over the c's such that

$$\sum_{j=0}^{N-1}|c_j|^2 = 1\,.$$

Observing (see [DiSj]), that

$$\int_{-\frac{NT}{2}}^{\frac{NT}{2}}|\psi_0^N(z)|^4\,dz = \int_{-\frac{T}{2}}^{\frac{T}{2}}\phi_1(z)^4\,dz + \widetilde{\mathcal{O}}(\exp -\frac{S}{2\epsilon})\,, \tag{7.4}$$

where ϕ_1 is the groundstate of the T-periodic problem, the minimum of this approximate functional, which is attained for $c_j = N^{-\frac{1}{2}}$, is

$$m_A^{N,(1)} = \lambda_{1,z} + \frac{\widehat{g}}{N}\int_{-\frac{NT}{2}}^{\frac{NT}{2}}|\psi_0^N(z)|^4\,dz\,. \tag{7.5}$$

So as a first approximation, we have obtained

Proposition 7.2.

$$m_A^{N,(0)}(\epsilon,\widehat{g}) = \lambda_{1,z} + \frac{\widehat{g}}{N}\Big(\int_{-\frac{NT}{2}}^{\frac{NT}{2}} |\psi_0^N(z)|^4\,dz\Big) + (\widehat{g}+1)\,\widetilde{\mathcal{O}}(\exp -\frac{S}{\epsilon})\,,$$

or

$$m_A^{N,(0)}(\epsilon,\widehat{g}) = \lambda_{1,z} + \frac{\widehat{g}}{N}\Big(\int_{-\frac{T}{2}}^{\frac{T}{2}} \phi_1(z)^4\,dz\Big) + \widehat{g}\,\widetilde{\mathcal{O}}(\exp -\frac{S}{2\epsilon}) + \widetilde{\mathcal{O}}(\exp -\frac{S}{\epsilon})\,. \quad (7.6)$$

The definition of $\widetilde{\mathcal{O}}$ is given in (1.28). If we apply this result to our context with $\widehat{g} = \omega_\perp g$, this yields information on the behavior of $m_A^{N,(0)}$ independently of Assumption (1.49).

7.1.4 Taking into account the tunneling

If we keep the main tunneling term, we get the following more accurate approximating functional

$$\begin{aligned}&\mathbb{C}^N \ni \mathbf{c} \mapsto \mathcal{E}_A^{N,\epsilon,\widehat{g},(2)}(c)\\ &\quad := \widehat{\lambda}_1\left(\textstyle\sum_{j=0}^{N-1}|c_j|^2\right) - \tau\Re\left(\textstyle\sum_{j=0}^{N-1} c_j\,\overline{c_{j+1}}\right) + \widehat{g}\,(\textstyle\sum_{j=0}^{N-1}|c_j|^4)\,(\int_{-\frac{NT}{2}}^{\frac{NT}{2}} |\psi_0^N(z)|^4\,dz)\,.\end{aligned} \quad (7.7)$$

Here τ is the hopping amplitude introduced around (3.12), $\widehat{\lambda}_1$ is the lowest eigenvalue corresponding to the Floquet condition $k=\frac{N}{2}$ for the linear problem on $]-\frac{T}{2},\frac{T}{2}[$, which is exponentially closed to λ_1 and we take the convention that $c_N = c_0$.
The quadratic form corresponds to the approximation in the first band :

$$\mathbb{C}^N \ni \mathbf{c} \mapsto \widehat{\lambda}_1\left(\sum_{j=0}^{N-1}|c_j|^2\right) - \tau\Re\left(\sum_{j=0}^{N-1} c_j\,\overline{c_{j+1}}\right) \quad (7.8)$$

which can be shown to be correct modulo $\widetilde{\mathcal{O}}(\exp -\frac{2S}{\epsilon})$.

Remark 7.3.
This time the minimizer could depend on $\widehat{g}$!! This is the kind of problem which is analyzed in [KMPS] and in Subsection 7.3.

Discussion about the justification of $\mathcal{E}_A^{N,\epsilon,\widehat{g},(2)}$
One can wonder why we forget some terms in the computation. Let us do this more carefully. To be consistent with what we forget in the linear case (terms of order $\mathcal{O}(\tau^2)$), we show first that one can approximate[8] $\left(\int_{-\frac{NT}{2}}^{\frac{NT}{2}} |\sum_{j=0}^{N-1} c_j\psi_j^N(z)|^4\, dz\right)$ by

$$
\begin{array}{l}
\left(\int_{-\frac{NT}{2}}^{\frac{NT}{2}} |\sum_{j=0}^{N-1} c_j\psi_j^N(z)|^4\, dz\right) = \\
\quad (\sum_{j=0}^{N-1} |c_j|^4)(\int_{-\frac{NT}{2}}^{\frac{NT}{2}} |\psi_0^N|^4 dz) \\
+\sum_{j=0}^{N-1} \Big((|c_j|^2+|c_{j+1}|^2)(c_j\,\overline{c_{(j+1)}}+c_{j+1}\,\overline{c_{(j)}})\,(\int_{-\frac{NT}{2}}^{\frac{NT}{2}} \psi_0^N(z)|\psi_0^N(z)|^2\cdot\psi_1^N(z)dz)\Big) \\
+\widetilde{\mathcal{O}}(\tau^2)\,.
\end{array}
\tag{7.9}
$$

This first approximation is based on the following lemma.

Lemma 7.4.

$$
\int_{-\frac{NT}{2}}^{\frac{NT}{2}} \psi_0^N(z)^2\psi_1^N(z)^2dz = \widetilde{\mathcal{O}}(\exp -\frac{2S}{\epsilon})\,.
$$

This is based on the property that, for all $\eta > 0$, there exists C_η such that

$$
|\psi_0^N(z)| \leq C_\eta \exp\frac{\eta}{h}\ \exp -\frac{1}{\epsilon}d_{Ag}^{mod}(z)\,, \tag{7.10}
$$

where $d_{Ag}^{mod}(z)$ is an even function such that

$$
d_{Ag}^{mod}(z,0) = 2\int_0^z \sqrt{\mathbf{w}(t)}\,dt\,,\quad \text{for } z\in[0,T[\,,
$$

and such that $d_{Ag}^{mod}(z,0)$ is increasing for $z\geq 0$.
On the contrary, this is a priori unclear[9] why one could forget terms like

$$
\widehat{\tau} = \widehat{g}\int_{-\frac{NT}{2}}^{\frac{NT}{2}} \psi_0^N(z)^3\psi_1^N(z)dz\,. \tag{7.11}
$$

(where we recall that $\mathbf{w}$ is even by Assumption (1.1) and that this implies ψ_0^N even and real). This term is a priori of the same order as τ. We have indeed

[8] We use here the assumption that the potential and hence ψ_0^N is even. We recall also that the ψ_j are real.

[9] In [KMPS], p. 5, between formulas (18) and (19), the term $\widehat{\tau}$ is discussed; see also p. 6 around formula (20).

Lemma 7.5.

$$\int_{-\frac{NT}{2}}^{+\frac{NT}{2}} \psi_0^N(z)^3\psi_1^N(z)\,dz = \widetilde{\mathcal{O}}(\exp -\frac{S}{\epsilon})\,. \tag{7.12}$$

Due to the decay estimates (7.10) for these (NT)- Wannier functions, the term to integrate in (7.12) decays like

$$\widetilde{\mathcal{O}}\left(\exp -\frac{1}{\epsilon}\left(3d_{Ag}^{mod}(z) + d_{Ag}^{mod}(z-T)\right)\right)\,,$$

so the main contribution comes from the origin and has the same size as $\exp -\frac{S}{\epsilon}$.

So it is necessary to be careful[10], if one wants to neglect $\widehat{\tau}$.

Let us now try to estimate $\int_{-\frac{NT}{2}}^{+\frac{NT}{2}} \psi_0^N(z)^3\psi_1^N(z)\,dz$ as $\epsilon \to 0$ more precisely. Heuristically, one can try to use a WKB approximation, this is available for ψ_0^N in the neighborhood of 0 but unfortunately, we do not have a good WKB approximation of $\psi_1^N(z)$ close to the origin, as observed in Subsection 3.3 (see (3.23)). So we have no obvious main term for the asymptotic behavior of $\int_{-\frac{NT}{2}}^{+\frac{NT}{2}} \psi_0^N(z)^3\psi_1^N(z)\,dz$. A reasonable guess (which is implicitly used by the physicists) should be to suggest the following conjecture.

Conjecture 7.6.

$$\widehat{\tau} = \widehat{g}\; o(\tau)\,, \tag{7.13}$$

as $\epsilon \to 0$.

The weaker mathematical result, which is obtained from Lemma 7.5 by the considerations above using Helffer-Sjöstrand techniques [DiSj], is the following proposition.

Proposition 7.7.
Under the assumption that there exists $\eta > 0$ *such that,*

$$0 \le \widehat{g}\exp\frac{\eta}{\epsilon} \le 1\,, \tag{7.14}$$

[10]We thank M. Snoek for kindly answering our questions on this problem.

then

$$m_A^{N,(0)} = m_A^{N,(2)} + o(\tau)\,. \tag{7.15}$$

holds.

This gives a motivation for the analysis of the DNLS model of [STKB] (with an extra term in $\lambda \sum_{j=0}^{N-1} |c_j|^2$).
If we consider the (NT)-periodic Floquet problem, we arrive naturally to questions analyzed in [KMPS] (16-17-18), and the remark after (21) in this paper.

7.2 On approximate models in case B : towards Snoek's model

Using the basis of the (NT)-Wannier approach), we can consider $\mathcal{E}_B^N$ introduced in (1.42) and consider the decomposition

$$\mathcal{E}_B^N(\psi_{0,\perp},\cdots,\psi_{N-1,\perp}) := \mathcal{E}_B^{N\,\prime}(\psi_{0,\perp},\cdots,\psi_{N-1,\perp}) + g||\sum_{j=0}^{N-1}\psi_j^N(z)\psi_{j,\perp}(x,y)||_{L^4}^4\,.$$

We now use various approximations related to the analysis of the z-problem ((NT)-Wannier functions). We get

$$\begin{array}{l}\mathcal{E}_B^{N\,\prime}(\psi_{0,\perp},\cdots,\psi_{N-1,\perp})\\ \quad\sim s\sum_{j=0}^{N-1}||\psi_{j,\perp}||^2 + t\sum_{j=0}^{N-1}\left(\langle\psi_{j,\perp},\psi_{j+1,\perp}\rangle + \langle\psi_{j,\perp},\psi_{j-1,\perp}\rangle\right)\,,\end{array}$$

and

$$g||\sum_{j=0}^{N-1}\psi_j(z)\psi_{j,\perp}(x,y)||_{L^4}^4 \sim g||\psi_0||_{L^4}^4\sum_{j=0}^{N-1}||\psi_{j,\perp}||_{L^4}^4\,.$$

So the approximate functional becomes

$$\begin{array}{ll}\mathcal{E}_B^{N,approx}((\psi_{j,\perp})_j) & = \sum_{j=0}^{N-1}\int_{\mathbb{R}^2}\left(\frac{1}{2}|\nabla\psi_{\perp,j}|^2 + V(x,y)|\psi_{j,\perp}(x,y)|^2\right)dxdy\\ & \quad +s\sum_{j=0}^{N-1}||\psi_{j,\perp}||^2\\ & \quad +t\sum_{j=0}^{N-1}\left(\langle\psi_{j,\perp},\psi_{j+1,\perp}\rangle + \langle\psi_{j,\perp},\psi_{j-1,\perp}\rangle\right)\\ & \quad +\widetilde{g}\sum_{j=0}^{N-1}||\psi_{j,\perp}||_{L^4}^4\,,\end{array} \tag{7.16}$$

which should be minimized over the $(\psi_{j,\perp})_j$ such that

$$\sum_{j=0}^{N-1} ||\psi_{j,\perp}||^2 = 1\,.$$

This is the model described by Snoek [Sn].

Starting from this model, one can, depending on the size of the various parameters, come back in some case to the situation when $(\psi_{j,\perp})_j$ is of the form $c_j\psi_\perp$, with $\sum_{j=0}^{N-1}|c_j|^2 = 1$. In this case, we come back to the results of the previous subsection. In the other cases, the problem seems completely open.

7.3 Spatial period-doubling in Bose-Einstein condensates in an optical lattice

Here we mainly follow [MNPS]. We look at the discrete model for which these authors refer to [STKB].

The Hamiltonian for the discrete model is formally defined[11] as

$$H(\mathbf{c}) = -\tau\sum_j(\overline{c_j}c_{j+1} + c_j\overline{c_{j+1}}) + I\sum_j|c_j|^4\,,$$

where $\mathbf{c} = (c_j) \in \ell^2(\mathbb{Z};\mathbb{C})$, $\tau \geq 0$, $I \geq 0$.

This is a particular case of the so-called *DNLS* model[12] (Discrete Non Linear Schrödinger model). But we will immediately reduce our analysis to the (NT)-periodic problem and Floquet variants of this problem.
We will restrict the sum above to $j = 1,\dots,N$, where N is a fixed positive integer. But for defining the tunneling term $(\overline{c_j}c_{j+1} + c_j\overline{c_{j+1}})$, we use the Floquet condition

$$c_{N+1} = \exp(ikN)\,c_1\,. \tag{7.17}$$

Remarks 7.8.

- *[MNPS] looks at the particular case $N = 2^p$.*

[11] after substraction of a term in the form $\sigma\sum_j|c_j|^2$,

[12] In the general case one should add the term $\sum_j\epsilon_j|c_j|^2$ when the trapping is present the authors propose $\epsilon_j = \tilde{\omega}j^2$ with $\tilde{\omega}$ proportional to ω_z.

- *When $k = 0$, this is the natural (NT)-periodic problem.*
- *Note that it is the standard Floquet problem only for $N = 1$.*
- *Note that we forget the term $\lambda \sum_j |c_j|^2$ which corresponds only to a shift of the energy.*

Hence we would like to minimize $H^{N,k}(\mathbf{c})$

$$H^{N,k}(\mathbf{c}) := -\tau \sum_{j=1}^{N} (\overline{c_j} c_{j+1} + c_j \overline{c_{j+1}}) + I \sum_{j=1}^{N} |c_j|^4 \,, \tag{7.18}$$

over the $\mathbf{c}$'s normalized in $\mathbb{C}^N$ by

$$||\mathbf{c}||^2 = N_c \,, \tag{7.19}$$

and the k-Floquet condition (7.17).
Moreover for future use we introduce the strictly positive parameter

$$\nu = N_c/N > 0 \,. \tag{7.20}$$

Remark 7.9.
In the preceding sections we were taking $N_c = 1$. Up to a change of the parameter τ, one can always reduce to the general case to this situation. A difference could occur if we take ν fixed and $N \to +\infty$.

We will then be interested in the analysis of the energy per particle

$$E(\tau, I, \nu, N, k) = \frac{1}{N_c} \inf_{||\mathbf{c}||^2 = N_c} H^{N,k}(\mathbf{c}) \,. \tag{7.21}$$

Writing

$$c_j = \exp i\, kj\ g_j \tag{7.22}$$

then from (7.17)

$$g_{1+N} = g_1 \,. \tag{7.23}$$

The case when $N = 1$ corresponds to the usual Floquet condition.
Writing that $\mathbf{c}$ is a critical value of $H^{N,k}$, we get that for some μ (which is called the chemical potential or the Lagrange multiplier in mathematics)

$$2I|c_j|^2 c_j - \tau\, (c_{j+1} + c_{j-1}) = \mu c_j \,, \tag{7.24}$$

for $j = 1, \ldots, N$, with condition (7.17). This becomes in terms of the g_j's

$$2I|g_j|^2 g_j - \tau\, (\exp ik\ g_{j+1} + \exp(-ik)\ g_{j-1}) = \mu g_j \,, \tag{7.25}$$

for $j = 1, \ldots, N$, with the N-periodic convention (7.23).

The case $N = 1$
In this case, we have simply one equation

$$2I|g_1|^2 g_1 - 2\tau\cos(k)\, g_1 = \mu\, g_1\,, \tag{7.26}$$

with

$$|g_1|^2 = \nu\,. \tag{7.27}$$

We find immediately that

$$\mu = -2\tau\cos(k) + 2I\nu \tag{7.28}$$

and

$$g_1 = \nu \exp i\phi_1\,. \tag{7.29}$$

The energy per particule E is then equal to

$$E = \frac{1}{N_c} H^{1,k}(\mathbf{c}) = -2\tau\cos(k) + I\nu\,. \tag{7.30}$$

For this choice of N, we have recovered exactly what we have found in the linear case $I = 0$. The effect of the non-linear term just creates a k-independent shift of the energy. Note also that as a function of k, the energy is minimal for $k = 0$, which is the periodic case.

The case $N = 2$
In this case, we get, using the periodicity assumption, the following system of equations

$$\begin{aligned} 2I|g_1|^2 g_1 - 2\tau\cos(k)\, g_2 = \mu g_1\,, \\ -2\tau\cos(k)\, g_1 + 2I|g_2|^2 g_2 = \mu g_2\,, \end{aligned} \tag{7.31}$$

with the normalization condition

$$|g_1|^2 + |g_2|^2 = N_c = 2\nu\,. \tag{7.32}$$

We write

$$g_j = |g_j| \exp i\varphi_j\,, \quad \text{for } j = 1, 2\,. \tag{7.33}$$

A suitable combination of the two lines gives

$$2I\left(|g_1|^2 - |g_2|^2\right) = 2\tau\cos(k)\left(\frac{|g_2|}{|g_1|}\exp i(\varphi_2 - \varphi_1) \;-\; \frac{|g_1|}{|g_2|}\exp -i(\varphi_2 - \varphi_1)\right)\,. \tag{7.34}$$

If we observe that the left hand side is real, we get

$$0 = 2\tau\cos(k)\left(\frac{|g_2|}{|g_1|} + \frac{|g_1|}{|g_2|}\right)\sin(\varphi_2 - \varphi_1)\,. \tag{7.35}$$

The real part of (7.34) is in any case given by

$$I\left(|g_1|^2 - |g_2|^2\right) = \tau\cos(k)\left(|g_2|^2 - |g_1|^2\right)\frac{1}{|g_1||g_2|}\cos(\varphi_2 - \varphi_1)\,. \tag{7.36}$$

We meet three cases.

Case 1
We first observe that the solutions corresponding to the case $N = 1$ are recovered by taking $\varphi_1 = \varphi_2$ and $|g_1| = |g_2|$.
Another family of solutions is obtained by taking $\varphi_1 = \varphi_2 + \pi$ and $|g_1| = |g_2|$. This corresponds to an "antiperiodic" solution over two periods.

The solutions such that $|g_1| = |g_2| = \sqrt{\nu}$ seem to be simply deformations of the case $I = 0$.
At least for I small, this is indeed also a consequence of the implicit function theorem when $\cos k \neq 0$.
The energy per particle E is the same as for $N = 1$.

Case 2
If we assume that

$$|g_1| \neq |g_2|\,, \tag{7.37}$$

and

$$\tau\cos k \neq 0\,, \tag{7.38}$$

then the previous necessary conditions become first

$$\sin(\varphi_2 - \varphi_1) = 0\,,$$

hence

$$\varphi_2 = \varphi_1\ mod(\mathbb{Z}\pi)\,,$$

and secondly (using the first one)

$$2I|g_1||g_2| = \pm 2\tau\cos k\,. \tag{7.39}$$

Using the normalization of g_1 and g_2, we get as a necessary condition

$$|\tau\cos k| \leq |I|\nu\,. \tag{7.40}$$

If these conditions are satisfied, we can find in function of the sign[13] of $\cos k$, a unique pair g_1, g_2 (up to a multiplication by $e^{i\theta}$). Coming back to the initial system of equations leads to the determination of μ which is given by

$$\mu = 4I\nu\,, \tag{7.41}$$

and of the energy E which is given by :

$$E = \frac{\tau^2}{I\nu}\cos^2 k \,+\, 2I\nu\,. \tag{7.42}$$

Case 3

It remains to consider the degenerate situation. If

$$\cos k = 0\,, \tag{7.43}$$

i.e. if

$$|k| = \frac{\pi}{2}\,, \tag{7.44}$$

Then

$$g_1 = \nu \exp i\varphi_1\,,\; g_2 = \nu \exp i\varphi_2\,, \tag{7.45}$$

is a solution for any pair (φ_1, φ_2). The corresponding μ is given by

$$\mu = 2I\nu\,, \tag{7.46}$$

and

$$E = I\nu\,. \tag{7.47}$$

This is the same energy that the one found for the usual Bloch state (with the same k) but note that the g_j are no more 1-periodic ($g_{j+1} \neq g_j$).

Question 7.10.

It is unclear in the discussion what is the status of k. Are we interested in minimizing over k? But in this case $k = 0$ and $N = 1$ seems optimal in the sense that they give the lowest E.

Remark 7.11.

An interesting problem, which is discussed in [MNPS], is the analysis of the stability, looking at the linearized corresponding problem.

Remark 7.12.

Of course the analysis of more general N's would be quite interesting. A few numerical results are given in [MNPS] corresponding to $N = 4$.

[13] It seems that in our problem we have $I \geq 0$ and $\tau > 0$.

8 Other optical lattices functionals

In this section, we discuss the choice of analyzing periodic boundary conditions in the z direction and the possibility of stating the problem differently. We compare the (NT)-periodic problem to the T-periodic problem and discuss shortly the question $N \to +\infty$.

8.1 Summary of the linear case

We summarize what we have obtained in the linear situation. Different techniques can be used for determining the bottom of the spectrum of H_z and then of H, but the ground state energies always coincide.

(i) Minimize the functional

$$\psi \mapsto Q(\psi) := \langle H_z \psi \mid \psi \rangle_{L^2(\mathbb{R})}\,, \tag{8.1}$$

over L^2-normalized ψ's in $C_0^\infty(\mathbb{R})$ (or in $H^1(\mathbb{R})$). In this case, the minimization gives the ground state energy but there is no minimizer in the form domain of the operator !

(ii) Minimize the functional

$$\psi \mapsto Q^{per}(\psi) = \int_{-\frac{T}{2}}^{+\frac{T}{2}} \left(\frac{1}{2} |\psi'(z)|^2 + W_\epsilon(z) |\psi(z)|^2 \right) dz\,, \tag{8.2}$$

over the L^2 normalized C^∞ T-periodic functions ψ's (or on $H^{1,per}$) . Here we integrate over one period ! The minimization will give the ground state energy of the periodic operator and the minimizer of the functional will be the ground state.

(iii) Minimize the functional

$$\psi \mapsto Q^{per,N}(\psi) = \int_{-\frac{NT}{2}}^{\frac{NT}{2}} \left(\frac{1}{2} |\psi'(z)|^2 + W_\epsilon(z) |\psi(z)|^2 \right) dz\,, \tag{8.3}$$

over the L^2-normalized C^∞ (NT)-periodic functions (or on $H^{1,N,per}$). Here we integrate over N periods ! The minimization will give the ground state energy of the periodic operator and the minimizer of the functional will be again the T-periodic ground state.

(iv) Minimize over $k \in [0, 2\pi/T[$, the infimum of the functional

$$Q^{Floq,k}(\psi) = \int_{-\frac{T}{2}}^{+\frac{T}{2}} \left(\frac{1}{2}|\psi'(z) - ik\psi(z)|^2 + W_\epsilon(z)|\psi(z)|^2 \right) dz \tag{8.4}$$

over the L^2-normalized C^∞ T-periodic functions ψ (or on $H^{1,per}$). Here we integrate over one period ! The minimization will give the ground state energy of the periodic operator (i.e. $k = 0$) and the minimizer of the functional will be the periodic ground state (corresponding to $k = 0$).

(v) Minimize over the space generated by the Wannier functions (identified with $\ell^2(\Gamma, \mathbb{C})$). This corresponds to the reduction to the first band and leads to the analysis of

$$\ell^2(\Gamma, \mathbb{C}) \ni \mathbf{c} = (c_\ell)_{\ell \in \Gamma} \mapsto \sum_{\ell, m} \widehat{\lambda}_1(\ell - m) c_\ell \overline{c_m}\,, \tag{8.5}$$

with $\sum_\ell |c_\ell|^2 = 1$.

(vi) Minimize over the space generated by the (NT)-Wannier functions (identified with $\ell^2(\Gamma^N, \mathbb{C}) = \mathbb{C}^N$). This corresponds to the reduction to the spectral space attached to the first N eigenfunctions of the (NT)-periodic problem living in the first band.

We emphasize, that, in each case, we get the same ground state energy.
As already mentioned, the 3-dimensional linear case introduced in (1.16) is easily reduced to the one-dimensional case H_z.

Remark 8.1.
The reader could be astonished that we discuss only the case $\omega_z = 0$. This is a current assumption in the physical literature. Mathematically, there is a dramatic change in the nature of the spectrum. The problem could become quite difficult in some regimes of ω_z and this will not discussed in this paper. Let us nethertheless make a few comments. When $\omega_z \neq 0$, the spectrum of H_z on the line becomes indeed discrete. By monotonicity, the bottom of the spectrum is above $\lambda_{1,z}$. One can also get an upper bound by computing the energy of a suitable quasimode (or more simply of the ground state of the linear problem) but this can only be good in some asymptotical regime.

8.2 The $3D$- functionals

Let us consider the fully non-linear problems and try to implement some of the results obtained for the linear models. We take $\omega_z = 0$, we have to analyze (see (1.1)) the functional

$$\Psi \mapsto Q_\Omega(\Psi) := \int_{\mathbb{R}^3} \left(\frac{1}{2} |(\nabla_{x,y,z} - i\Omega \times r)\Psi(\mathbf{r})|^2 + (V(\mathbf{r}) + W_\epsilon(z) - \frac{1}{2}\Omega^2 r^2)|\Psi(\mathbf{r})|^2 + g|\Psi(\mathbf{r})|^4 \right) dxdydz \,. \tag{8.6}$$

We denote by $\mathcal{D}_\Omega$ the natural maximal form domain of the form $Q_\Omega(\Psi)$ in $L^2(\mathbb{R}^3)$, that is

$$\mathcal{D}_\Omega = \{u \in H^1(\mathbb{R}^3)\,,\, xu \in L^2(\mathbb{R}^3)\,,\, yu \in L^2(\mathbb{R}^3)\} \,. \tag{8.7}$$

We denote the intersection of the $L^2(\mathbb{R}^3)$-unit ball with $\mathcal{D}_\Omega$:

$$\mathcal{S}_\Omega = \{\Psi \in \mathcal{D}_\Omega\,,\, ||\Psi||_{L^2} = 1\} \,.$$

We call the infimum of this functional

$$E_\Omega := \inf_{\Psi \in \mathcal{S}_\Omega} Q_\Omega(\Psi) \,. \tag{8.8}$$

Because there is no harmonic trapping in the z-variable the choice of the condition of normalization in $L^2(\mathbb{R}^3)$ is questionable.

The T-periodicity of the optical lattice in the z-variable suggests to consider other functionals, where we integrate over $\mathbb{R}^2_{x,y} \times] - \frac{T}{2}, \frac{T}{2}[$ (or more intrinsically over $\mathbb{R}^2_{x,y} \times (\mathbb{R}/T\mathbb{Z})$), or over $\mathbb{R}^2_{x,y} \times] - \frac{NT}{2}, \frac{NT}{2}[$ for some integer N, and where the variational space has to be defined suitably (periodic conditions or Floquet conditions). We refer to Subsection 8.1, for the discussion done in the linear case. In the non-linear case, this has led to the introduction of the "periodic" Bose-Einstein functional (see (1.15)) We will denote by $Q_\Omega^{per,N}$ the functional obtained by integration over N periods (see (1.10)). We call $\mathcal{D}_{BE}^{per}$, the natural maximal form domain of the form Q_Ω^{per}. It corresponds to the distributions Ψ in $H^1_{loc}(\mathbb{R}^3)$, satisfying (1.13) and such that, the restriction Ψ_T to $\mathbb{R}^2_{x,y} \times] - \frac{T}{2}, \frac{T}{2}[$, satisfies :

$$\Psi_T \in H^1(\mathbb{R}^2_{x,y} \times] - \frac{T}{2}, \frac{T}{2}[)\,,\ \sqrt{x^2+y^2}\, \Psi_T \in L^2(\mathbb{R}^2_{x,y} \times] - \frac{T}{2}, \frac{T}{2}[) \,. \tag{8.9}$$

We note that this functional has clearly a minimizer in $\mathcal{S}_\Omega^{per}$, where

$$\mathcal{S}_\Omega^{per} = \{\Psi \in \mathcal{D}_\Omega^{per}\,,\ \int_{\mathbb{R}^2_{x,y}\times]-\frac{T}{2},\frac{T}{2}[} |\Psi(x,y,z)|^2\, dxdydz = 1\,\}. \tag{8.10}$$

We denote this infimum by

$$E_\Omega^{per} = \inf_{\Psi\in\mathcal{S}_\Omega^{per}} Q_\Omega^{per}(\Psi)\,. \tag{8.11}$$

In the spirit of the Floquet theory, one can also be interested in the analysis of the Floquet Bose-Einstein family of functionals, defined for $k \in \mathbb{R}$ by :

$$\begin{aligned}\Psi \mapsto\ & Q_{\Omega,k}^{Floq}(\Psi)\\ := & \int_{\mathbb{R}^2_{x,y}\times]-\frac{T}{2},\frac{T}{2}[} \Big(\tfrac{1}{2}|(\nabla_{x,y} - i\Omega r_\perp)\Psi|^2 - \tfrac{1}{2}\Omega^2 r^2|\Psi|^2\\ & +\tfrac{1}{2}|(\partial_z + ik)\Psi|^2 + (V(\mathbf{r}) + W_\epsilon(z))|\Psi|^2\Big)\, dxdydz\\ & +g\int_{\mathbb{R}^2_{x,y}\times]-\frac{T}{2},\frac{T}{2}[} |\Psi|^4\, dxdydz\,,\end{aligned} \tag{8.12}$$

where Ψ satisfies

$$\Psi(x,y,z+T) = \Psi(x,y,z)\,. \tag{8.13}$$

We call $\mathcal{D}_{\Omega,k}^{Floq}$, the natural maximal form domain of $Q_{\Omega,k}^{Floq}$, which is actually independent of k and Ω :

$$\mathcal{D}_{\Omega,k}^{Floq} = \mathcal{D}_\Omega^{per}\,.$$

We note that we have here a family over k of functionals. Each of these functionals has a minimizer in S_k^{Floq}, where

$$\mathcal{S}_{\Omega,k}^{Floq} =: \{\Psi \in \mathcal{D}_{\Omega,k}^{Floq}\,,\ \int_{\mathbb{R}^2_{x,y}\times]-\frac{T}{2},\frac{T}{2}[} |\Psi|^2\, dxdydz = 1\,\}. \tag{8.14}$$

It is natural to be interested in the quantity

$$E_\Omega^{Floq} := \inf_k E_{\Omega,k}^{Floq}\,, \tag{8.15}$$

with

$$E_{\Omega,k}^{Floq} := \inf_{\Psi\in\mathcal{S}_{\Omega,k}^{Floq}} Q_{\Omega,k}^{Floq}(\Psi)\,. \tag{8.16}$$

Remark 8.2.
In the physics literature, this corresponds to a ground state of a condensate at rest in the frame of the optical lattice. The energies $E_{\Omega,k}^{Floq}$ describe states of the system where all the atoms move with respect to the optical potential, at fixed velocity, giving rise to a constant current equal to k. Experimentally, this is achieved by moving the optical lattice with respect to the condensate. We refer to [KMPS] and the references therein.

We would like to compare the various functionals.

Because $g \geq 0$, all the functional are bounded from below, admit an infimum and a lower bound is given by the analysis of the linear problem corresponding to $g = 0$. But there is probably no existence of a minimizer for the Bose Einstein functional. So we will have to consider minimizing sequences or approximate minimizers using possibly other models having minimizers. We refer for this to Subsection 8.1. The new point is now that it is unclear that the various ground state energies obtained by the different procedures coincide !

Finally, it could be interesting to compare directly the infimum of the three functionals above and then to find good approximations of these infima.

At the moment we have shown in the "linear" section that :

$$E_\Omega(g=0) = E_\Omega^{per}(g=0) = E_\Omega^{Floq}(g=0) = \inf \sigma(H_\Omega) = \lambda_{1,z} + \omega_\perp \,. \quad (8.17)$$

We have also mentioned, observing the monotonicity of the functionals with respect to g, that, for $g \geq 0$,

$$\begin{aligned} & E_\Omega(g=0) \leq E_\Omega(g)\,, \\ & E_\Omega^{per}(g=0) \leq E_\Omega^{per}(g)\,, \\ \text{and} \quad & E_\Omega^{Floq}(g=0) \leq E_\Omega^{Floq}(g)\,. \end{aligned} \quad (8.18)$$

This is further developed in Proposition 8.3.

8.3 Comparison between the Floquet Bose-Einstein functionals and the periodic Bose-Einstein functional

The argument which follows is only correct when $\Omega = 0$. The idea is that using the Kato inequality, one has

$$Q_{BE}^{per}(|\psi|) \leq Q_k^{Floq}(\psi)\,,\ \forall k \quad (8.19)$$

In the periodic case, the minimization over complex functions leads to the same infimum as in the real case.
We then obtain

$$E^{Floq} \leq E^{per} \leq E_k^{Floq}\,, \quad (8.20)$$

hence

$$E^{Floq} = E^{per}\,. \quad (8.21)$$

This seems to suggest that, when $\Omega = 0$, there is no interest to introduce Floquet conditions, if one is only interested in the determination of the ground state energy.

8.4 Comparison between the periodic Bose-Einstein functional and the Bose-Einstein functional on $\mathbb{R}^3$

Here we again work for general Ω's satisfying (1.5). We can naturally try what was working in the linear case. If $\Psi^{per}(x,y,z) = \psi_{per}(x,y)\varphi_1(z)$ is the periodic minimizer of the linear problem, i.e. satisfying

$$H^\Omega \Psi^{per} = E^{lin}\Psi^{per}\,,\ ||\Psi^{per}||^2_{L^2(\mathbb{R}^2_{x,y}\times]-\frac{T}{2},\frac{T}{2}[)} = 1$$

and

$$\Psi^{per}(x,y,z+T) = \Psi^{per}(x,y,z)\,, \tag{8.22}$$

with $E^{lin} = \omega_\perp + \lambda_{1,z}$, we can use as trial function for the Bose Einstein functional

$$\widetilde{\Psi}_R := c_R\chi_R(z)\Psi^{per}(x,y,z)\,, \tag{8.23}$$

where $c_R > 0$ is determined by the condition

$$c_R^2 \int_{\mathbb{R}^3} |\chi_R(z)\Psi^{per}(x,y,z)|^2\, dxdydz = 1\,, \tag{8.24}$$

Here $R \geq 1$ is a free parameter which will tend to $+\infty$ and χ_R is a function with support in $[-RT-T, RT+T]$ equal to 1 on $[-RT,+RT]$ whose first derivative is independent of $R \geq 1$.
It is immediate to see, from the normalization chosen for Ψ^{per}, that

$$c_R \sim \frac{1}{\sqrt{2R}}\,,\quad \text{as } R \to +\infty\,. \tag{8.25}$$

We note that these trial functions are radial in the (x,y) variable and are independent of Ω.

The main point is to observe that we have

$$\begin{aligned}\textstyle\int_{\mathbb{R}^3} |\widetilde{\Psi}_R(x,y,z)|^4\, dxdydz &\sim 2Rc_R^4 \textstyle\int_{\mathbb{R}^2\times]-\frac{T}{2},\frac{T}{2}[} |\Psi^{per}(x,y,z)|^4\, dxdydz\\ &\sim \tfrac{1}{2R}\textstyle\int_{\mathbb{R}^2\times]-\frac{T}{2},\frac{T}{2}[} |\Psi^{per}(x,y,z)|^4\, dxdydz\,.\end{aligned} \tag{8.26}$$

Hence

$$\lim_{R\to+\infty}\int_{\mathbb{R}^3} |\widetilde{\Psi}_R(x,y,z)|^4\, dxdydz = 0\,, \tag{8.27}$$

We also obtain easily that, as $R \to +\infty$,

$$\lim_{R\to+\infty}\int_{\mathbb{R}^3} |(\nabla - i\Omega\times\mathbf{r})\widetilde{\Psi}_R(x,y,z)|^2 = \int_{\mathbb{R}^2\times]-\frac{T}{2},\frac{T}{2}[} |(\nabla - i\Omega\times\mathbf{r})\Psi^{per}(x,y,z)|^2\, dxdydz \tag{8.28}$$

and

$$\lim_{R\to+\infty}\int_{\mathbb{R}^3}(V(x,y,z)-\frac{1}{2}\Omega^2r^2)|\widetilde{\Psi}_R(x,y,z)|^2$$

$$=\int_{\mathbb{R}^2\times]-\frac{T}{2},\frac{T}{2}[}(V(x,y,z)-\frac{1}{2}\Omega^2r^2)|\Psi^{per}(x,y,z)|^2\,dxdydz\,. \quad (8.29)$$

So we obtain that

$$\lim_{R\to+\infty}Q_\Omega(\widetilde{\Psi}_R)=E_\Omega^{per}(g=0)\,. \quad (8.30)$$

One can also observe that everything is actually Ω independent.

Combining with what we have verified for the linear case, we obtain that, for $g\geq 0$,

$$E_\Omega^{per}(g=0)=E(g=0)\leq E_\Omega(g)\leq\lim_{R\to+\infty}Q_\Omega(\widetilde{\Psi}_R)=E_\Omega^{per}(g=0)\,. \quad (8.31)$$

So we have proved the

Proposition 8.3.
For all $g\geq 0$, all $0\leq\Omega<\omega_\perp$,

$$E(g)=E_\Omega(g)=E_\Omega^{per}(g=0)=E_\Omega(g=0)=E(g=0)\,. \quad (8.32)$$

The conclusion is that if we look at the Bose-Einstein functional on $\mathbb{R}^3$ the infimum of the functional restricted to L^2-normalized states is independent of $g\geq 0$ and Ω and is immediately obtained by the ground state energy of the Hamiltonian attached to the case $g=0$ and $\Omega=0$.

The result is of course also valid for the 1-dimensional problem and is independent of any asymptotic analysis.

Remark 8.4.
Another natural physical problem would be to analyze the quantity

$$\liminf_{N_c\to+\infty}\frac{1}{N_c}\left(\inf_{\int_{-\frac{NT}{2}}^{+\frac{NT}{2}}|\Psi|^2\,dx=N_c}Q_\Omega^{per,N}(\Psi)\right)$$

or

$$\limsup_{N_c \to +\infty} \frac{1}{N_c} \left(\inf_{\int_{-\frac{NT}{2}}^{+\frac{NT}{2}} |\Psi|^2 \, dx = N_c} Q_\Omega^{per,N}(\Psi) \right)$$

where we compute the energy by integrating over N periods and where

$$N_c/N = \nu$$

(ν fixed). Upper bounds for this model are the periodic models with g replaced by $g\nu$. We met already this problem in Subsection 7.3 for discrete models.

8.5 Comparison between the (NT)-periodic problem and the T-problem

In this subsection, we pursue the analysis of the links between the (NT)-periodic problem ($N > 1$) and the T-periodic problem. We recall from Subsubsection 2.2.3 that, for the (NT)-periodic problem in $1D$, the ground state energy is $\lambda_{1,z}$. Moreover, in the semi-classical regime we have a packet of N eigenvalues which are exponentially close separated from the $(N+1)$-th eigenvalue by a splitting δ_z^N which satisfies (1.27). In case A, a natural question is :

Question 8.5.
Is the minimizer of $\mathcal{E}_A^N$ T-periodic as in the linear case ?

When the answer is yes, we immediately obtain that

$$m_A^N(\epsilon, \widehat{g}) = m_A(\epsilon, \frac{\widehat{g}}{N}) \tag{8.33}$$

and we can directly use what we have done for proving Theorem 1.3 by replacing g by $\frac{g}{N}$.
To our knowledge the answer to this question is unknown, so it is natural to look at simpler models.

In case B a natural question could be

Question 8.6.
Is the corresponding minimizer in this reduced space T-periodic ?

When the answer to this question is yes, we have seen in (6.4) together with the discussion around (5.43) (with the additional assumption that the minimizer is periodic) that

$$m_{B,\Omega}^{N} = m_{B,\Omega}(\frac{\widetilde{g}}{N})\,.$$

We could then use what we have used for the proof of Theorem 1.5. This should work in the case when g and Ω are small.

Actually, we could have asked more directly the following question

Question 8.7.
Under which condition on g and Ω is the minimizer of the (NT)-periodic initial problem T-periodic ?

If it is the case, we get immediately

$$E_{\Omega}^{per,N}(g) = E_{\Omega}^{per}(\frac{g}{N}) \tag{8.34}$$

So we can directly relate the treatment of the (NT)-periodic problem to our preceding studies, without any use of (NT)-periodic Wannier functions.

The general answer is unknown. One suspects by bifurcation arguments that it is true for g and Ω small enough, but the physicists seem to wait for the other situation. This should in particular be the case for sufficiently large rotation Ω (see for example [CorR-DY]) or in the case with (NT)-Floquet conditions (see the discussion in Subsection 7.3 on an approximating model).

A Floquet theory

We follow the presentation of [DiSj] (p. 160-161), who are actually dealing with a more complicate situation. If we take as lattice $\Gamma = \mathbb{Z}T$, the dual lattice Γ^* is $\Gamma^* = \frac{2\pi}{T}\mathbb{Z}$. For $u \in \mathcal{S}(\mathbb{R})$ and $k \in \mathbb{R}$, we put

$$\mathcal{U}u(y;k) = \sum_{\gamma\in\Gamma} \exp i\gamma\, k\;\; u(y-\gamma)\,. \tag{A.1}$$

We notice that $\mathcal{U}u(y;k)$ only depends on k modulo the dual lattice Γ^* so $\mathbb{U}u(y;k)$ is well defined on $\mathbb{R}\times(\mathbb{R}/\Gamma^*)$.

For $k \in \mathbb{R}/\Gamma^*$, we put

$$\mathcal{D}'_k = \{u \in \mathcal{D}'(\mathbb{R}) \; ; \; u(y+\gamma) = \exp i\gamma\, k \;\, u(y)\} \,, \tag{A.2}$$

and

$$\mathcal{H}_k = \{u \in L^2_{loc}(\mathbb{R}) \cap \mathcal{D}'_k \; ; \; \int_E |u(y)|^2 \, dy < +\infty\} \,, \tag{A.3}$$

where E is a fundamental domain of Γ (for example $E = [-\frac{T}{2}, \frac{T}{2}[$).
When $k = 0$, $\mathcal{H}_0$ denotes simply the space of T-periodic functions in $L^2_{loc}(\mathbb{R})$.
From (A.1) we see that

$$\mathcal{U}u(\,\cdot\,; k) \in \mathcal{H}_k \,, \tag{A.4}$$

and if we view $\mathcal{H}_k$ as a bundle over $\mathbb{R}/\Gamma^*$, we can view $\mathcal{U}u$ as a section of this bundle. We write $\mathcal{U}u \in C^\infty(\mathbb{R}/\Gamma^*; \mathcal{H}_k)$.

Now, if $v \in L^2(\mathbb{R}/\Gamma^*)$, one can expand it in a Fourier series :

$$v(k) = \sum_{\gamma \in \Gamma} \widehat{v}(\gamma) \, \exp i\gamma\, k \,, \tag{A.5}$$

where

$$\widehat{v}(\gamma) = \frac{T}{2\pi} \int_0^{\frac{2\pi}{T}} \exp -i\gamma\, k \;\, v(k) \, dk \,. \tag{A.6}$$

We have the Parseval formula

$$\frac{T}{2\pi} \int_0^{\frac{2\pi}{T}} |v(k)|^2 \, dk = \sum_{\gamma \in \Gamma} |\widehat{v}(\gamma)|^2 \,. \tag{A.7}$$

Now, for any $y \in \mathbb{R}$, we can view (A.1) as the Fourier expansion of $\mathcal{U}(y; \cdot)$, so (A.7) gives

$$\frac{T}{2\pi} \int_0^{\frac{2\pi}{T}} |\mathcal{U}u(y;k)|^2 \, dk = \sum_{\gamma \in \Gamma} |u(y-\gamma)|^2 \,. \tag{A.8}$$

Integrating over $y \in [-\frac{T}{2}, \frac{T}{2}]$, we get

$$\frac{T}{2\pi} \int_{-\frac{T}{2}}^{\frac{T}{2}} \left(\int_0^{\frac{2\pi}{T}} |\mathcal{U}u(y;k)|^2 \, dk \right) dy = \sum_{\gamma \in \Gamma} \int_{-\frac{T}{2}}^{\frac{T}{2}} |u(y-\gamma)|^2 \, dy = \int_{-\infty}^{+\infty} |u(y)|^2 \, dy \,. \tag{A.9}$$

So $\mathcal{U}$ can be extended to an isometry from $L^2(\mathbb{R})$ into $L^2(\mathbb{R}/\Gamma^*;\mathcal{H}_k)$, which, as an Hilbert space, can be also described as the space of the v's in $L^2_{loc}(\mathbb{R}^2)$ such that

$$\left\{\begin{array}{ll} v(y+\gamma;k) = \exp i\gamma\, k\ \ v(y;k)\,, & \forall \gamma\in\Gamma\,,\\ v(y;k+\gamma^*) = v(y;k)\,, & \forall\gamma^*\in\Gamma^*\,,\end{array}\right. \tag{A.10}$$

with the norm, whose square appears in the left hand side of (A.9), i.e.

$$v\mapsto \sqrt{\int_{[-\frac{T}{2},\frac{T}{2}]\times[0,2\pi/T]} |v(y;k)|^2\, dy\, dk}\,. \tag{A.11}$$

Like in the standard analysis of the Fourier transform, we have now to analyze the surjectivity property and the construction of an inverse.
If $(y,k)\mapsto v(y;k)$ belongs to $C^\infty(\mathbb{R}/\Gamma^*;\mathcal{H}_k)$, we can write the Fourier expansion of v with respect to the second variable :

$$v(y;k) = \sum_{\gamma\in\Gamma} \widehat{v}_\gamma(y)\ \exp i\gamma\, k\,, \tag{A.12}$$

with

$$\widehat{v}_\gamma(y) = \frac{T}{2\pi}\int_0^{\frac{2\pi}{T}} \exp -i\gamma\, k\ \ v(y;k)\, dk\,. \tag{A.13}$$

Using the first line of (A.10), we see that

$$\widehat{v}_\gamma(y) = \widehat{v}_0(y-\gamma)\,. \tag{A.14}$$

Hence, when v is smooth, we have

$$v = \mathcal{U}\mathcal{W}v\,, \tag{A.15}$$

where

$$\mathcal{W}v(y) = \frac{T}{2\pi}\int_0^{\frac{2\pi}{T}} v(y;k)\, dk = \widehat{v}_0(y)\,. \tag{A.16}$$

Using (A.16), (A.14) and (A.12), we obtain

$$\begin{array}{ll} ||\mathcal{W}v||^2_{L^2(\mathbb{R})} & = \sum_{\gamma\in\Gamma}\int_{-\frac{T}{2}}^{\frac{T}{2}} |\widehat{v}_0(y-\gamma)|^2\, dy\\ & = \sum_{\gamma\in\Gamma}\int_{-\frac{T}{2}}^{\frac{T}{2}} |\widehat{v}_\gamma(y)|^2\, dy\\ & = ||v||^2_{L^2(\mathbb{R}/\Gamma^*,\mathcal{H}_k)}\,. \end{array} \tag{A.17}$$

This shows that $\mathcal{W}$ is an isometry of $L^2(\mathbb{R}/\Gamma^*;\mathcal{H}_k)$ into $L^2(\mathbb{R})$. Hence $\mathcal{W}$ is a bounded right inverse for $\mathcal{U}$. Since $\mathcal{U}$ is an isometry, we conclude that $\mathcal{U}$ is

unitary and that its inverse is $\mathcal{W}$.
Now, when considering $P := -\frac{d^2}{dy^2} + W(y)$ with W T-periodic, we see that

$$\mathcal{U}P\mathcal{U}^{-1} = \int_{[0,2\pi/T]}^{\oplus} \widetilde{P}_k \, dk \,, \tag{A.18}$$

where, by definition the right hand side in (A.18) denotes the selfadjoint operator Q on $L^2(\mathbb{R}/\Gamma^*; \mathcal{H}_k)$, with domain $L^2(\mathbb{R}/\Gamma^*; \mathcal{H}_k^2)$, which is given by

$$Qv(y;k) = \left(\widetilde{P}_k v(\cdot\,;k)\right)(y) \,. \tag{A.19}$$

Here above

$$\mathcal{H}_k^2 = \{u \in \mathcal{H}_k \,,\; u^{(\ell)} \in \mathcal{H}_k \;\text{ for } |\ell| \leq 2\} \,,$$

and $\widetilde{P}_k$ is the selfadjoint operator on $\mathcal{H}_k$ associated to the differential operator $-\frac{d^2}{dy^2} + W(y)$ with domain $\mathcal{H}_k^2$.
Finally, we note that for $k \in \mathbb{R}/\Gamma^*$, $\widetilde{P}_k$ is unitary equivalent to the operator

$$P_k = \exp -iy\,k \;\circ \widetilde{P}_k \;\circ \exp iy\,k \,, \tag{A.20}$$

which is now acting on $\mathcal{H}_0$ (corresponding to the T-periodic fuunctions in L^2_{loc}). More explicitly it takes the form

$$P_k = -\left(\frac{d}{dy} + ik\right)^2 + W(y) \,.$$

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